The Lie–Trotter splitting method for nonlinear evolutionary problems involving critical parameters. An exact local error representation and application to nonlinear Schrödinger equations in the semi-classical regime.

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Abstract In the present work, we investigate the error behaviour of exponential operator splitting methods for nonlinear evolutionary problems of the form

$$u'(t) = A\big(u(t)\big) + B\big(u(t)\big)\,, \quad 0 \leq t \leq T\,, \qquad u(0) \text{ given}\,.$$

In particular, our concern is to deduce an exact local error representation that is suitable in the presence of critical parameters. Essential tools in the theoretical analysis including time-dependent nonlinear Schrödinger equations in the semi-classical regime as well as parabolic initial-boundary value problems with high spatial gradients are an abstract formulation of differential equations on function spaces and the formal calculus of Lie-derivatives. We expose the general mechanism on the basis of the least technical example method, the first-order Lie–Trotter splitting.

Our conjecture that exponential operator splitting methods are favourable for the time integration of a nonlinear Schrödinger equation in the semi-classical regime, provided that the time stepsizes are suitably chosen in dependence of the magnitude of the critical parameter $0 < \varepsilon \ll 1$, is confirmed by a numerical example for the time-dependent Gross–Pitaevskii equation

$$\begin{aligned} \mathrm{i}\,\varepsilon\,\partial_t \psi(x,t) &= -\tfrac{1}{2}\,\varepsilon^2 \Delta\,\psi(x,t) + U(x)\,\psi(x,t) + \vartheta\,\big|\psi(x,t)\big|^2\,\psi(x,t)\,, \\ \psi(x,0) &\text{ given}\,, \qquad x \in \mathbb{R}^d\,, \quad 0 \leq t \leq T\,, \end{aligned}$$

and substantiated by theoretical considerations for the Lie–Trotter splitting method. Moreover, we illustrate the ability of an embedded 4(3) splitting pair to serve as a reliable basis for a local error control.

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1 Introduction

In this work, our concern is to investigate the error behaviour of exponential operator splitting methods for the time integration of abstract nonlinear evolutionary problems

$$\begin{cases} u'(t) = A\big(u(t)\big) + B\big(u(t)\big)\,, \quad 0 \leq t \leq T\,, \\ u(0) \text{ given}\,, \end{cases} \tag{1.1}$$

see [2,5–8,11,15,17–19,22–24,26,27,30]. In particular, our objective is the derivation of an exact local error representation that is well-suited in the presence of unbounded nonlinear operators and critical parameters. A most useful tool to this purpose is the formal calculus of Lie-derivatives, which is suggestive of the less involved linear case [8–10].

In comparison with other local error expansions for splitting methods that are based on the Baker–Campbell–Hausdorff formula or on techniques exploited in [13, 19,20,22,25,30] in the context of time-dependent Schrödinger equations, the approach presented allows to capture correctly the error behaviour of time-splitting methods for nonlinear evolutionary problems involving unbounded nonlinear operators and critical parameters. Therefore, our theoretical analysis applies to time-dependent nonlinear Schrödinger equations in the semi-classical regime as well as to nonlinear parabolic initial-boundary value problems with high spatial gradients.

As a model problem, we consider the following time-dependent nonlinear Schrödinger equation for $\psi : \mathbb{R}^d \times [0,T] \to \mathbb{C} : (x,t) \mapsto \psi(x,t)$

$$\begin{cases} \mathrm{i}\,\varepsilon\,\partial_t \psi(x,t) = -\frac{1}{2}\,\varepsilon^2 \Delta\,\psi(x,t) + U(x)\,\psi(x,t) + \vartheta\,\big|\psi(x,t)\big|^2\,\psi(x,t)\,, \\ \psi(x,0) \text{ given}\,, \qquad x \in \mathbb{R}^d\,, \quad 0 \leq t \leq T\,, \end{cases} \tag{1.2}$$

with (small) parameter $\varepsilon > 0$, real-valued external potential $U : \mathbb{R}^d \to \mathbb{R}$, and coupling constant $\vartheta \in \mathbb{R}$, imposing asymptotic boundary conditions on the unbounded domain. The above problem is related to the time-dependent Gross–Pitaevskii equation [14,28] which arises in the description of the macroscopic wave function of a Bose–Einstein condensate. Employing an abstract formulation of ordinary differential equations on function spaces, the initial-boundary value problem (1.2) takes the form (1.1) with unbounded linear operator A comprising the Laplacian (and part of the potential) and unbounded nonlinear multiplication operator B involving (part of) the potential and the cubic nonlinearity.

The incentive for this work originates from the question whether exponential operator splitting methods are favourable for nonlinear evolutionary Schrödinger equations in the semi-classical regime; our interest in this theme is inspired by theoretical

and numerical investigations for the first-order Lie–Trotter splitting and the second-order Strang splitting provided by [3,4,12], see also the references given therein.

Numerical comparisons given in [2,5,7,27], e.g., for nonlinear Schrödinger equations such as (1.2) with $\varepsilon = 1$ show that higher-order splitting schemes are superior to standard integrators when low tolerances are required or long-term integrations are carried out. These numerical observations are also confirmed by theoretical investigations. For instance, for an exponential operator splitting method of (classical) order p, applied to a linear evolutionary Schrödinger equation involving a sufficiently regular bounded potential, the local error expansion exploited in [19,30] leads to an error estimate of the form

$$\left\|u_N - u(t_N)\right\|_{L^2} \leq C \left(\left\|u_0 - u(0)\right\|_{L^2} + \sum_{n=0}^{N-1} h_n^{p+1} \left\|u(0)\right\|_{H^p} \right).$$

In [20], in the context of the multi-configuration time-dependent Hartree–Fock equations, the techniques used in [13,19,22,25,30] are extended to establish estimates for high-order splitting methods applied to nonlinear evolutionary problems; main tools in the error analysis are the formal calculus of Lie-derivatives and bounds for Lie-commutators of the involved nonlinear operators.

However, for small parameter values $0 < \varepsilon \ll 1$, the above mentioned approach is *not* appropriate to provide optimal (local) error bounds with respect to ε; thus, different techniques are needed for a better theoretical understanding of the error behaviour of exponential operator splitting methods for nonlinear evolutionary problems and the dependence of the admissible temporal stepsize on the critical parameter. In our previous work [10], which is concerned with an exact local error representation for splitting methods applied to linear equations, we followed an alternative approach. In particular, for linear Schrödinger equations and classical Wentzel–Kramers–Brillouin initial values that satisfy the condition $\varepsilon^j \|u(0)\|_{H^j} \leq M_j$ with a constant $M_j > 0$ for $1 \leq j \leq p$, the convergence estimate

$$\left\|u_N - u(t_N)\right\|_{L^2} \leq \left\|u_0 - u(0)\right\|_{L^2} + C \frac{h^p}{\varepsilon}, \qquad h = \max_{0 \leq n \leq N-1} h_n,$$

results with constant $C > 0$ depending on M_j, $0 \leq j \leq p$, $\left\|\partial_x^j U\right\|_{L^\infty}$, $1 \leq j \leq 2p$, and the end time t_N; the dependence of the global error on the time stepsize and the critical parameter is also confirmed by numerical examples.

In the present paper, we extend the error analysis of [10] for linear equations to nonlinear problems (1.1). In order to illustrate the general mechanism, we focus on the first-order Lie–Trotter splitting method

$$\begin{cases} u_n = \mathrm{e}^{h_{n-1} D_A} \, \mathrm{e}^{h_{n-1} D_B} \, u_{n-1}, \quad 1 \leq n \leq N, \\ u_0 \text{ given}, \end{cases} \tag{1.3}$$

yielding numerical approximations to the exact solution values at time grid points $0 = t_0 < t_1 < \cdots < t_N \leq T$ with associated stepsizes $h_{n-1} = t_n - t_{n-1}$, $1 \leq n \leq N$. In this case, it is evident that our approach leads to a compact exact local error representation, which is advantageous for further investigations in regard to nonlinear

Schrödinger equations such as (1.2). Indeed, the defect operator of the Lie–Trotter splitting method (1.3) possesses the representation

$$\begin{aligned} \mathscr{L}(t,v) &= \mathrm{e}^{tD_A}\,\mathrm{e}^{tD_B}\,v - \mathrm{e}^{D_{A+B}}v \\ &= \int_0^t \int_0^{\tau_1} \mathrm{e}^{\tau_1 D_A}\,\mathrm{e}^{\tau_2 D_B}\,\big[D_A,D_B\big]\,\mathrm{e}^{(\tau_1-\tau_2)D_B}\,\mathrm{e}^{(t-\tau_1)D_{A+B}}\,v\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1\,; \end{aligned} \tag{1.4}$$

especially, for linear operators A and B the above formula reduces to

$$\begin{aligned} \mathscr{L}(t,v) &= \big(\mathrm{e}^{tB}\,\mathrm{e}^{tA} - \mathrm{e}^{t(A+B)}\big)\,v \\ &= \int_0^t \int_0^{\tau_1} \mathrm{e}^{(t-\tau_1)(A+B)}\,\mathrm{e}^{(\tau_1-\tau_2)B}\,\big[B,A\big]\,\mathrm{e}^{\tau_2 B}\,\mathrm{e}^{\tau_1 A}\,v\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1\,. \end{aligned}$$

Relations such as (1.4) provide the basis for a convergence analysis of exponential operator splitting methods when applied to nonlinear evolution equations.

The structure of this work is as follows. In Section 2, we state the abstract nonlinear evolutionary problem and specify the considered exponential operator splitting methods. Section 3 is devoted to the derivation of an appropriate local error representation; we give a detailed derivation involving marginal technicalities for the first-order Lie–Trotter splitting method and indicate the generalisation to high-order methods. We first deduce the statement of Theorem 1 by employing standard techniques and notations and then comment on a formal extension of the linear case using the calculus of Lie-derivatives. Applications to nonlinear Schrödinger equations in the semi-classical regime are the contents of Section 4. Theoretical considerations, also confirmed by numerical illustrations, imply that the Lie–Trotter splitting method is favourable for the time integration of the one-dimensional Gross–Pitaevskii equation, provided that the time stepsizes are chosen sufficiently small; in case of a regular initial condition with bounded spatial derivatives, independent of the critical parameter $0 < \varepsilon \ll 1$, time stepsizes of the magnitude of ε are needed, whereas for an initial condition in classical Wentzel–Kramers–Brillouin form time stepsizes sufficiently smaller than the critical parameter are required. For higher-order exponential operator splitting methods, improved accuracy properties are observed. Furthermore, as the shape of the solution to the Gross–Pitaevskii equation suggests an adaptive time stepsize selection, we illustrate the ability of an embedded 4(3) splitting pair to serve as a reliable basis for an adaptive time stepsize selection.

As in the present work the focus is on the least technical example method, the first-order Lie–Trotter splitting method, we favour standard notations revealing the non-trivial auxiliary results to the formal calculus of Lie-derivatives. Formal calculations are carried out under the tacit requirement that the arising unbounded operators and compositions thereof are well-defined on suitably chosen domains and time intervals.

2 Splitting methods for nonlinear evolutionary problems

2.1 Nonlinear evolutionary problems

In the present work, we consider an initial value problem of the form

$$\begin{cases} u'(t) = F\big(u(t)\big)\,, \quad 0 \le t \le T\,, \\ u(0) \text{ given}\,, \end{cases} \tag{2.1a}$$

where the structure of the unbounded nonlinear operator $F : D(F) \subset X \to X$ suggests a decomposition into two parts

$$F(v) = A(v) + B(v)\,, \qquad v \in D(A) \cap D(B)\,, \tag{2.1b}$$

with unbounded nonlinear operators $A : D(A) \subset X \to X$ and $B : D(B) \subset X \to X$; throughout, we tacitly require that the domains are suitably chosen subspaces of the underlying Banach space $(X, \|\cdot\|_X)$ such that $D(F) = D(A) \cap D(B) \neq \emptyset$.

The exact solution of the evolutionary problem (2.1) is (formally) given by

$$u(t) = \mathscr{E}_F\big(t, u(0)\big)\,, \qquad 0 \le t \le T\,, \tag{2.2a}$$

with evolution operator $\mathscr{E}_F$ depending on the actual time and the initial value; as the differential equation in (2.1a) is supposed to be autonomous, we may neglect the dependence on the initial time. Besides, we employ the formal notation

$$u(t) = \mathrm{e}^{tD_F} u(0)\,, \qquad 0 \le t \le T\,, \tag{2.2b}$$

which is suggestive of the (less involved) linear case. Here, the evolution operator e^{tD_F} and the Lie-derivative D_F associated with F are given by

$$\mathrm{e}^{tD_F} G\, v = G\big(\mathscr{E}_F(t, v)\big)\,, \quad 0 \le t \le T\,, \qquad D_F\, G\, v = G'(v)\, F(v)\,, \tag{2.3a}$$

for any unbounded nonlinear operator $G : D(G) \subset X \to X$ with Fréchet derivative G'; whenever G is the identity operator, we write

$$\mathrm{e}^{tD_F} v = \mathscr{E}_F(t, v)\,, \quad 0 \le t \le T\,, \qquad D_F\, v = F(v)\,, \tag{2.3b}$$

for short. We note that the relation

$$D_F = \tfrac{\mathrm{d}}{\mathrm{d}t}\big|_{t=0}\, \mathrm{e}^{tD_F}$$

holds, since $\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}_F(t, v) = F\big(\mathscr{E}_F(t, v)\big)$ and $\mathscr{E}_F(0, v) = v$ and thus by the chain rule

$$\begin{aligned} \tfrac{\mathrm{d}}{\mathrm{d}t}\big|_{t=0}\, \mathrm{e}^{tD_F} G\, v &= \tfrac{\mathrm{d}}{\mathrm{d}t}\big|_{t=0}\, G\big(\mathscr{E}_F(t, v)\big) = G'\big(\mathscr{E}_F(t, v)\big)\, F\big(\mathscr{E}_F(t, v)\big)\big|_{t=0} = G'(v)\, F(v) \\ &= D_F\, G\, v\,; \end{aligned}$$

this is in accordance with the identity $L = \frac{\mathrm{d}}{\mathrm{d}t}|_{t=0}\, \mathrm{e}^{tL}$, valid for instance for any bounded linear operator $L : X \to X$ with the exponential function defined by the power series.

2.2 Exponential operator splitting methods

The nonlinear evolutionary problem (2.1) is discretised in time by an exponential operator splitting method of (classical) order $p \geq 1$ involving $s \geq 1$ compositions. We employ the following general formulation of a splitting method that includes various example methods proposed in literature.

Starting from an initial value $u_0 \approx u(0)$, numerical approximations u_n to the exact solution values $u(t_n)$ at time grid points $0 = t_0 < t_1 < \cdots < t_N \leq T$ with associated time stepsizes $h_{n-1} = t_n - t_{n-1}$, $1 \leq n \leq N$, are determined through a recurrence relation of the form

$$\begin{cases} u_n = \mathscr{S}(h_{n-1}, u_{n-1}), \quad 1 \leq n \leq N, \\ u_0 \text{ given}; \end{cases} \tag{2.4a}$$

the splitting operator $\mathscr{S}$ is defined through

$$\mathscr{S}(t,v) = \mathrm{e}^{a_1 t D_A} \, \mathrm{e}^{b_1 t D_B} \cdots \mathrm{e}^{a_s t D_A} \, \mathrm{e}^{b_s t D_B} v, \qquad 0 \leq t \leq T, \tag{2.4b}$$

with (real or complex) method coefficients $(a_j, b_j)_{j=1}^s$, see also (2.3). We meanwhile suppose the procedure (2.4) to be well-defined on a certain function space.

Low-order example methods that can be cast into the scheme (2.4) are the first-order Lie–Trotter splitting method, where

$$p = s = 1, \qquad a_1 = b_1 = 1, \tag{2.5}$$

see also (1.3), and the widely used second-order symmetric Lie–Trotter or Strang splitting method, where

$$p = s = 2, \qquad a_1 = a_2 = \tfrac{1}{2}, \quad b_1 = 1, \quad b_2 = 0, \tag{2.6}$$

see [29,31]. Evidently, when exchanging the roles of the operators A and B, the Lie–Trotter splitting and the Strang splitting method are cast into the general form (2.4) with $s = 2$ and $a_1 = b_2 = 0$, $a_2 = b_1 = 1$ or $a_1 = 0$, $a_2 = 1$, $b_1 = b_2 = \frac{1}{2}$, respectively.

A fourth-order method involving four compositions by Yoshida [15, p. 40, Formula (4.4)], i.e., $p = s = 4$, possesses the real coefficients

$$\begin{gathered} a_1 = 0, \quad a_2 = a_4 = \gamma_1 = \tfrac{1}{2 - \sqrt[3]{2}}, \quad a_3 = \gamma_2 = -\tfrac{\sqrt[3]{2}}{2 - \sqrt[3]{2}}, \\ b_1 = b_4 = \tfrac{1}{2}\gamma_1, \quad b_2 = b_3 = \tfrac{1}{2}(\gamma_1 + \gamma_2). \end{gathered} \tag{2.7}$$

Further example methods of higher-order that were proposed in literature are reviewed in [15,24], see also [10,25,30] and the references given therein. The coefficients of a favourable fourth-order splitting method proposed in [6] and a related third-order splitting method constructed in [21] in are displayed in Table 2.1.

j	a_j	j	b_j
1	0	1,7	0.0829844064174052
2,7	0.245298957184271	2,6	0.3963098014983680
3,6	0.604872665711080	3,5	−0.0390563049223486
4,5	$\frac{1}{2}-(a_2+a_3)$	4	$1-2(b_1+b_2+b_3)$
j	$\hat{a}_j$	j	$\hat{b}_j$
1	a_1	1	b_1
2	a_2	2	b_2
3	a_3	3	b_3
4	a_4	4	b_4
5	0.3752162693236828	5	0.4463374354420499
6	1.4878666594737946	6	−0.0060995324486253
7	−1.3630829287974774	7	0

Table 2.1 Coefficients $(a_j,b_j)_{j=1}^7$ of a fourth-order splitting method proposed in [6] (top). Coefficients $(\hat{a}_j,\hat{b}_j)_{j=1}^7$ of a related third-order splitting method (bottom).

3 An exact local error representation

In the following, we deduce an appropriate representation of the defect operator

$$\begin{aligned}\mathscr{L}(t,v) &= \mathscr{S}(t,v)-\mathscr{E}_F(t,v)\\ &= \mathrm{e}^{a_1 tD_A}\,\mathrm{e}^{b_1 tD_B}\cdots\,\mathrm{e}^{a_s tD_A}\,\mathrm{e}^{b_s tD_B}\,v-\mathrm{e}^{tD_F}v\,,\qquad 0\le t\le T\,,\end{aligned}\tag{3.1}$$

of an exponential operator splitting method (2.4); the local error representation remains valid for problems (2.1) involving unbounded nonlinear operators and is well-suited in the presence of critical parameters. In Section 3.1, we give a detailed depiction for the first-order Lie–Trotter splitting method (2.5) involving marginal technicalities and then indicate the generalisation to high-order methods utilising a formal extension of the linear case by the calculus of Lie-derivatives; to keep the presentation tight, several auxiliary results are collected in Section 3.2.

Below, we employ the following notations. The Lie-commutator of two nonlinear operators G and H is defined through

$$\big[G,H\big](v) = G'(v)\,H(v)-H'(v)\,G(v)\,;\tag{3.2a}$$

clearly, for linear operators G and H, due to $G'(v)=G$ as well as $H'(v)=H$, the above relation reduces to $\big[G,H\big](v)=\big[G,H\big]\,v=(GH-HG)\,v$. In accordance with (3.2a), we further set

$$\big[D_G,D_H\big]\,v = D_G D_H\,v - D_H D_G\,v\,,\tag{3.2b}$$

see (2.3) for the definition of the Lie-derivative; note that $\big[D_G,D_H\big]\,v=-\big[G,H\big](v)$.

3.1 Lie–Trotter splitting method

For the Lie–Trotter splitting method (2.5), the splitting operator (2.4b) simplifies to

$$\mathscr{S}(t,v) = \mathscr{E}_B\big(t,\mathscr{E}_A(t,v)\big)\,,\qquad 0\le t\le T\,.\tag{3.3}$$

In regard to the primal initial value problem

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathscr{E}_F(t,v) = F\big(\mathscr{E}_F(t,v)\big)\,, \quad 0 \le t \le T\,, \\ \mathscr{E}_F(0,v) = v\,, \end{cases} \tag{3.4}$$

see also (2.1) and (2.2), we determine the time derivative of (3.3) and rewrite it as follows

$$\begin{aligned} \tfrac{\mathrm{d}}{\mathrm{d}t}\,\mathscr{S}(t,v) &= B\Big(\mathscr{E}_B\big(t,\mathscr{E}_A(t,v)\big)\Big) + \partial_2\mathscr{E}_B\big(t,\mathscr{E}_A(t,v)\big)\,A\big(\mathscr{E}_A(t,v)\big) \\ &= F\big(\mathscr{S}(t,v)\big) + \partial_2\mathscr{E}_B\big(t,\mathscr{E}_A(t,v)\big)\,A\big(\mathscr{E}_A(t,v)\big) - A\big(\mathscr{S}(t,v)\big)\,; \end{aligned}$$

consequently, we obtain the initial value problem

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathscr{S}(t,v) = F\big(\mathscr{S}(t,v)\big) + R(t,v)\,, \quad 0 \le t \le T\,, \\ \mathscr{S}(0,v) = v\,, \end{cases} \tag{3.5a}$$

which involves the time-dependent remainder

$$R(t,v) = \partial_2\mathscr{E}_B\big(t,\mathscr{E}_A(t,v)\big)\,A\big(\mathscr{E}_A(t,v)\big) - A\big(\mathscr{S}(t,v)\big)\,, \qquad 0 \le t \le T\,. \tag{3.5b}$$

In order to relate the solutions of the initial value problems (3.4) and (3.5), we apply the nonlinear variation-of-constants formula, see Theorem 2; this yields the following relation for the defect operator

$$\mathscr{L}(t,v) = \int_0^t \partial_2\mathscr{E}_F\big(t-\tau_1,\mathscr{S}(\tau_1,v)\big)\,R(\tau_1,v)\,\mathrm{d}\tau_1\,, \qquad 0 \le t \le T\,,$$

see (3.1). Furthermore, by Lemma 1 we obtain the identity

$$\begin{aligned} R(\tau_1,v) &= \partial_2\mathscr{E}_B\big(\tau_1,\mathscr{E}_A(\tau_1,v)\big)\,A\big(\mathscr{E}_A(\tau_1,v)\big) - A\Big(\mathscr{E}_B\big(\tau_1,\mathscr{E}_A(\tau_1,v)\big)\Big) \\ &= \int_0^{\tau_1} \partial_2\mathscr{E}_B\big(\tau_1-\tau_2,\mathscr{E}_A(\tau_1,v)\big) \\ &\qquad\qquad \times \big[B,A\big]\Big(\mathscr{E}_B\big(\tau_2,\mathscr{E}_A(\tau_1,v)\big)\Big)\,\mathrm{d}\tau_2\,, \qquad 0 \le \tau_1 \le t \le T\,, \end{aligned}$$

see also (3.2) and (3.5b). Altogether, the above considerations imply the following local error representation; for a justification of the compact formal notation, we apply Lemma 2 with $G_1 = H_1 = A$, $G_2 = G_3 = H_2 = B$, $G_4 = F$, $t_\ell = \tau_\ell$, $\ell = 1,2$, $t_3 = \tau_1 - \tau_2$, and $t_4 = t - \tau_1$, see also (2.3).

Theorem 1 (Local error representation, Lie–Trotter splitting) *For the nonlinear evolutionary problem* (2.1) *the defect operator* (3.1) *of the first-order Lie–Trotter splitting method* (2.5) *possesses the integral representation*

$$\begin{aligned} \mathscr{L}(t,v) &= \int_0^t \int_0^{\tau_1} \mathrm{e}^{\tau_1 D_A}\,\mathrm{e}^{\tau_2 D_B}\big[D_A,D_B\big]\,\mathrm{e}^{(\tau_1-\tau_2)D_B}\,\mathrm{e}^{(t-\tau_1)D_F}\,v\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1 \\ &= \int_0^t \int_0^{\tau_1} \partial_2\mathscr{E}_F\big(t-\tau_1,\mathscr{S}(\tau_1,v)\big)\;\partial_2\mathscr{E}_B\big(\tau_1-\tau_2,\mathscr{E}_A(\tau_1,v)\big) \\ &\qquad\qquad \times \big[B,A\big]\Big(\mathscr{E}_B\big(\tau_2,\mathscr{E}_A(\tau_1,v)\big)\Big)\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1\,, \qquad 0 \le t \le T\,. \end{aligned}$$

Remark 1 In accordance with [10], for initial value problems (2.1) involving unbounded linear operators the local error representation of Theorem 1 reduces to

$$\mathscr{L}(t,v) = \int_0^t \int_0^{\tau_1} \mathrm{e}^{(t-\tau_1)(A+B)}\, \mathrm{e}^{(\tau_1-\tau_2)B} \big[B,A\big]\, \mathrm{e}^{\tau_2 B} \mathrm{e}^{\tau_1 A} v \,\mathrm{d}\tau_2 \,\mathrm{d}\tau_1 \,, \qquad 0 \le t \le T \,.$$

Simplistically, replacing the operators A and B by the associated Lie-derivatives D_A and D_B and reversing the order, the result for the nonlinear case is obtained.

Remark 2 A rigorous extension of the exact local error representation for the first-order Lie–Trotter splitting method to higher-order splitting methods and the investigation for a particular application is left for future work; in this case, it is indispensable to employ the formal calculus of Lie-derivatives. However, it is expected that exact local error representation for high-order exponential operator splitting methods formally resembles the relation for the linear case [10] replacing A and B by the associated Lie-derivatives and reversing the sequence of the involved operators.

3.2 Auxiliary results

In this section, we collect several auxiliary results that are needed for the derivation of our local error representation for exponential operator splitting methods (2.4) applied to nonlinear evolutionary problems (2.1).

In the following, we let $G : D(G) \subset X \to X$ and $H : D(H) \subset X \to X$ denote unbounded nonlinear operators (with suitably chosen domains). In regard to (2.1), we consider the evolutionary problem

$$\begin{cases} v'(t) = G\big(v(t)\big)\,, \quad 0 \le t \le T\,, \\ v(0) = v_0\,, \end{cases}$$

with exact solution formally given by $v(t) = \mathscr{E}_G(t, v_0)$ for $0 \le t \le T$, see also (2.2). We recall that the evolution operator $\mathscr{E}_G$ and its derivative with respect to the initial value, which we denote by $\partial_2 \mathscr{E}_G$, fulfill the initial value problems

$$\begin{aligned} &\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\, \mathscr{E}_G(t,v_0) = G\big(\mathscr{E}_G(t,v_0)\big)\,, \quad 0 \le t \le T\,, \\ \mathscr{E}_G(0,v_0) = v_0\,, \end{cases} \\ &\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\, \partial_2 \mathscr{E}_G(t,v_0) = G'\big(\mathscr{E}_G(t,v_0)\big)\, \partial_2 \mathscr{E}_G(t,v_0)\,, \quad 0 \le t \le T\,, \\ \partial_2 \mathscr{E}_G(t,v_0)\big|_{t=0} = I\,. \end{cases} \end{aligned} \tag{3.6}$$

Clearly, the evolution operator $\mathscr{E}_G$ satisfies

$$\mathscr{E}_G(t+s,v_0) = \mathscr{E}_G\big(s,\mathscr{E}_G(t,v_0)\big) = \mathscr{E}_G\big(t,\mathscr{E}_G(s,v_0)\big)\,, \qquad 0 \le t+s \le T\,;$$

more generally, in the context parabolic equations the above relation holds true under the additional restriction $s,t \ge 0$. As a consequence, the identity

$$\begin{aligned} \partial_2 \mathscr{E}_G(t,v_0)\, G(v_0) &= \tfrac{\mathrm{d}}{\mathrm{d}s}\big|_{s=0}\, \mathscr{E}_G\big(t,\mathscr{E}_G(s,v_0)\big) = \tfrac{\mathrm{d}}{\mathrm{d}s}\big|_{s=0}\, \mathscr{E}_G(t+s,v_0) \\ &= G\big(\mathscr{E}_G(t,v_0)\big)\,, \qquad 0 \le t \le T\,, \end{aligned} \tag{3.7}$$

follows.

An essential tool for the derivation of our local error representation is the nonlinear variation-of-constants formula.

Theorem 2 (Gröbner–Alekseev formula) *The analytical solutions of the following initial value problems*

$$\begin{cases} v'(t) = H\big(t, v(t)\big) = G\big(v(t)\big) + R\big(t, v(t)\big)\,, \quad 0 \le t \le T\,, \\ v(0) = v_0\,, \end{cases}$$

$$\begin{cases} v'(t) = G\big(v(t)\big)\,, \quad 0 \le t \le T\,, \\ v(0) = v_0\,, \end{cases}$$

are related through the nonlinear variation-of-constants formula

$$\begin{aligned} \mathscr{E}_H(t, v_0) &= \mathscr{E}_G(t, v_0) \\ &\quad + \int_0^t \partial_2 \mathscr{E}_G\big(t-\tau, \mathscr{E}_H(\tau, v_0)\big)\, R\big(\tau, \mathscr{E}_H(\tau, v_0)\big)\, \mathrm{d}\tau\,, \qquad 0 \le t \le T\,. \end{aligned}$$

Proof With the help of relation (3.7), we obtain

$$\begin{aligned} &\tfrac{\mathrm{d}}{\mathrm{d}\tau}\, \mathscr{E}_G\big(t-\tau, \mathscr{E}_H(\tau, v_0)\big) \\ &\quad = -\, G\Big(\mathscr{E}_G\big(t-\tau, \mathscr{E}_H(\tau, v_0)\big)\Big) \\ &\qquad + \partial_2 \mathscr{E}_G\big(t-\tau, \mathscr{E}_H(\tau, v_0)\big)\, H\big(\tau, \mathscr{E}_H(\tau, v_0)\big) \\ &\quad = -\, G\Big(\mathscr{E}_G\big(t-\tau, \mathscr{E}_H(\tau, v_0)\big)\Big) \\ &\qquad + \partial_2 \mathscr{E}_G\big(t-\tau, \mathscr{E}_H(\tau, v_0)\big)\, G\big(\mathscr{E}_H(\tau, v_0)\big) \\ &\qquad\quad + \partial_2 \mathscr{E}_G\big(t-\tau, \mathscr{E}_H(\tau, v_0)\big)\, R\big(\tau, \mathscr{E}_H(\tau, v_0)\big) \\ &\quad = \partial_2 \mathscr{E}_G\big(t-\tau, \mathscr{E}_H(\tau, v_0)\big)\, R\big(\tau, \mathscr{E}_H(\tau, v_0)\big)\,, \qquad 0 \le \tau \le t \le T\,; \end{aligned}$$

therefore, the desired result follows at once from

$$\begin{aligned} \mathscr{E}_H(t, v_0) - \mathscr{E}_G(t, v_0) &= \mathscr{E}_G\big(0, \mathscr{E}_H(t, v_0)\big) - \mathscr{E}_G\big(t, \mathscr{E}_H(0, v_0)\big) \\ &= \mathscr{E}_G\big(t-\tau, \mathscr{E}_H(\tau, v_0)\big)\big|_{\tau=0}^{t} \\ &= \int_0^t \tfrac{\mathrm{d}}{\mathrm{d}\tau}\, \mathscr{E}_G\big(t-\tau, \mathscr{E}_H(\tau, v_0)\big)\, \mathrm{d}\tau \\ &= \int_0^t \partial_2 \mathscr{E}_G\big(t-\tau, \mathscr{E}_H(\tau, v_0)\big)\, R\big(\tau, \mathscr{E}_H(\tau, v_0)\big)\, \mathrm{d}\tau\,, \quad 0 \le t \le T\,. \end{aligned}$$

We note that for the non-autonomous problem involving H, the associated evolution operator $\mathscr{E}_H$ depends on the actual time, the initial time, and the initial value; in this case, we write $\mathscr{E}_H(t, v_0) = \mathscr{E}_H(t, 0, v_0)$ for short. □

In particular, for G a time-independent (unbounded) linear operator generating a semi-group $\big(\mathrm{e}^{tG}\big)_{t \ge 0}$, we retain the linear variation of constants formula

$$\mathscr{E}_H(t, v_0) = \mathrm{e}^{tG} v_0 + \int_0^t \mathrm{e}^{(t-\tau)G}\, R\big(\tau, \mathscr{E}_H(\tau, v_0)\big)\, \mathrm{d}\tau\,, \qquad 0 \le t \le T\,,$$

since $\mathscr{E}_G(t,v_0) = \mathrm{e}^{tG}v_0$ and thus $\partial_2\mathscr{E}_G(t,\cdot) = \mathrm{e}^{tG}$, see also [11,17,18,23,26].

In order to further expand terms of the form (3.5b), we apply the following auxiliary result; we refer to (3.2) for the definition of the Lie-commutator.

Lemma 1 *For unbounded nonlinear operators G and H, the identity*

$$\begin{aligned}\partial_2\mathscr{E}_G\big(t,v\big)\,H(v) - H\big(\mathscr{E}_G(t,v)\big)\\ = \int_0^t \partial_2\mathscr{E}_G(t-\tau,v)\,\big[G,H\big]\big(\mathscr{E}_G(\tau,v)\big)\,\mathrm{d}\tau\,, \qquad 0\le t\le T\,,\end{aligned}$$

holds true.

Proof In accordance with (3.5b), we set $R(t,v) = \partial_2\mathscr{E}_G\big(t,v\big)\,H(v) - H\big(\mathscr{E}_G(t,v)\big)$ for a fixed element v and $0\le t\le T$. Rewriting the time derivative of R as

$$\begin{aligned}\tfrac{\mathrm{d}}{\mathrm{d}t}R(t,v) &= G'\big(\mathscr{E}_G(t,v)\big)\;\partial_2\mathscr{E}_G(t,v)\,H(v) - H'\big(\mathscr{E}_G(t,v)\big)\;G\big(\mathscr{E}_G(t,v)\big)\\ &= G'\big(\mathscr{E}_G(t,v)\big)\;R(t,v)\\ &\qquad + G'\big(\mathscr{E}_G(t,v)\big)\;H\big(\mathscr{E}_G(t,v)\big) - H'\big(\mathscr{E}_G(t,v)\big)\;G\big(\mathscr{E}_G(t,v)\big)\,, \quad 0\le t\le T\,,\end{aligned}$$

see (3.6), and using $R(0,v) = \partial_2\mathscr{E}_G(0,v)\,H(v) - H\big(\mathscr{E}_G(0,v)\big) = 0$ thus yields the linear initial value problem

$$\begin{cases} \tfrac{\mathrm{d}}{\mathrm{d}t}R(t,v) = G'\big(\mathscr{E}_G(t,v)\big)\,R(t,v) + \big[G,H\big]\big(\mathscr{E}_G(t,v)\big)\,, \quad 0\le t\le T\,,\\ R(0,v) = 0\,,\end{cases}$$

see also (3.2) and (3.6); we note that the evolution operator of the associated homogeneous linear differential equation is given by $\partial_2\mathscr{E}_G(t,v)$. As a consequence, the (linear variant of the) variation-of-constants formula implies the given result, see also Theorem 2. □

We next reformulate the composition that arises in the local error representation of the Lie–Trotter splitting by utilising the formal calculus of Lie-derivatives, see (2.3).

Lemma 2 *For nonlinear operators G_j, $1\le j\le 4$, and H_j, $1\le j\le 2$, the following relation*

$$\begin{aligned}&\mathrm{e}^{t_1D_{G_1}}\,\mathrm{e}^{t_2D_{G_2}}\,\big[D_{H_1},D_{H_2}\big]\,\mathrm{e}^{t_3D_{G_3}}\,\mathrm{e}^{t_4D_{G_4}}\,v_0\\ &\qquad = \partial_2\mathscr{E}_{G_4}\big(t_4,\mathscr{E}_{G_3}(t_3,v)\big)\;\partial_2\mathscr{E}_{G_3}(t_3,v)\,\big[H_2,H_1\big](v)\big|_{v=\mathscr{E}_{G_2}(t_2,\mathscr{E}_{G_1}(t_1,v_0))}\end{aligned}$$

is valid.

Proof We consider the composition

$$L_1(v) = \mathrm{e}^{t_3D_{G_3}}\,\mathrm{e}^{t_4D_{G_4}}\,v = \mathscr{E}_{G_4}\big(t_4,\mathscr{E}_{G_3}(t_3,v)\big)$$

and determine its Fréchet derivative

$$L_1'(v) = \partial_2\mathscr{E}_{G_4}\big(t_4,\mathscr{E}_{G_3}(t_3,v)\big)\;\partial_2\mathscr{E}_{G_3}(t_3,v)\,.$$

Fig. 4.1 (top left)	$\omega = 1$	$\vartheta = 1$	$\partial_x \sigma_0 \neq 0$	$h = h_0$	$\alpha \approx -1$
Fig. 4.1 (top right)	$\omega = 1$	$\vartheta = 1$	$\partial_x \sigma_0 \neq 0$	$h = \varepsilon$	$\alpha \approx p$
Fig. 4.2 (top left)	$\omega = 1$	$\vartheta = 1$	$\sigma_0 = 0$	$h = h_0$	$\alpha \approx -1$
Fig. 4.2 (top right)	$\omega = 1$	$\vartheta = 1$	$\sigma_0 = 0$	$h = \varepsilon$	$\alpha \approx 2 \lfloor p + \frac{1}{2} \rfloor$
Fig. 4.1 (bottom left)	$\omega = 1$	$\vartheta = 0$	$\partial_x \sigma_0 \neq 0$	$h = h_0$	$\alpha = -1$
Fig. 4.1 (bottom right)	$\omega = 1$	$\vartheta = 0$	$\partial_x \sigma_0 \neq 0$	$h = \varepsilon$	$\alpha = p$
Fig. 4.2 (bottom left)	$\omega = 1$	$\vartheta = 0$	$\sigma_0 = 0$	$h = h_0$	$\alpha = -1$
Fig. 4.2 (bottom right)	$\omega = 1$	$\vartheta = 0$	$\sigma_0 = 0$	$h = \varepsilon$	$\alpha = 2 \lfloor p + \frac{1}{2} \rfloor$
Fig. 4.3 (top left)	$\omega = 0$	$\vartheta = 1$	$\partial_x \sigma_0 \neq 0$	$h = h_0$	$\alpha \approx -1$
Fig. 4.3 (top right)	$\omega = 0$	$\vartheta = 1$	$\partial_x \sigma_0 \neq 0$	$h = \varepsilon$	$\alpha \approx p$
Fig. 4.3 (bottom left)	$\omega = 0$	$\vartheta = 1$	$\sigma_0 = 0$	$h = h_0$	$\alpha \approx -1$
Fig. 4.3 (bottom right)	$\omega = 0$	$\vartheta = 1$	$\sigma_0 = 0$	$h = \varepsilon$	$\alpha \approx 2 \lfloor p + \frac{1}{2} \rfloor$

Table 4.1 Time integration of problem (4.2) with initial condition (4.3) ($\partial_x \sigma_0 \neq 0$) or (4.4) ($\sigma_0 = 0$), respectively, by various splitting methods of orders $1 \leq p \leq 4$. Observed dependence $\mathscr{O}(\varepsilon^\alpha)$ of the dominant local error term on the critical parameter ε within the chosen range of h/ε.

Moreover, due to the fact that

$$L_{1+j}(v) = D_{H_j} \, \mathrm{e}^{t_3 D_{G_3}} \, \mathrm{e}^{t_4 D_{G_4}} \, v = L_1'(v) H_j(v) \,, \qquad j = 1,2 \,,$$
$$L_{1+j}'(v) = L_1''(v) H_j(v) + L_1'(v) H_j'(v) \,, \qquad j = 1,2 \,,$$

a straightforward calculation yields the relation

$$L_4(v) = \big[D_{H_1}, D_{H_2} \big] \, \mathrm{e}^{t_3 D_{G_3}} \, \mathrm{e}^{t_4 D_{G_4}} \, v = L_3'(v) H_1(v) - L_2'(v) H_2(v) = L_1'(v) \big[H_2, H_1 \big](v) \,.$$

Using that

$$L_5(v) = \mathrm{e}^{t_2 D_{G_2}} \big[D_{H_1}, D_{H_2} \big] \, \mathrm{e}^{t_3 D_{G_3}} \, \mathrm{e}^{t_4 D_{G_4}} \, v = L_4\big(\mathscr{E}_{G_2}(t_2, v) \big)$$

and as a consequence

$$\mathrm{e}^{t_1 D_{G_1}} \, \mathrm{e}^{t_2 D_{G_2}} \big[D_{H_1}, D_{H_2} \big] \, \mathrm{e}^{t_3 D_{G_3}} \, \mathrm{e}^{t_4 D_{G_4}} \, v = L_5\big(\mathscr{E}_{G_1}(t_1, v) \big) \,,$$

the statement follows. □

4 Nonlinear Schrödinger equations in the semi-classical regime

In this section, we discuss the ability of the exact local error representation of Theorem 1 to provide optimal local error estimates for the first-order Lie–Trotter splitting method (2.5) when applied to time-dependent nonlinear Schrödinger equations in the semi-classical regime. In Section 4.1, we give a numerical example for the Gross–Pitaevskii equation (1.2) which illustrates and confirms the theoretical considerations of Section 4.2. We believe that in both, the numerical example and the theoretical considerations, it gives insight to draw a comparison with the less involved linear case treated in our previous work [10].

For simplicity, we henceforth focus on a model problem in a single space dimension; for our purposes, this restriction is adequate and considerably facilitates the

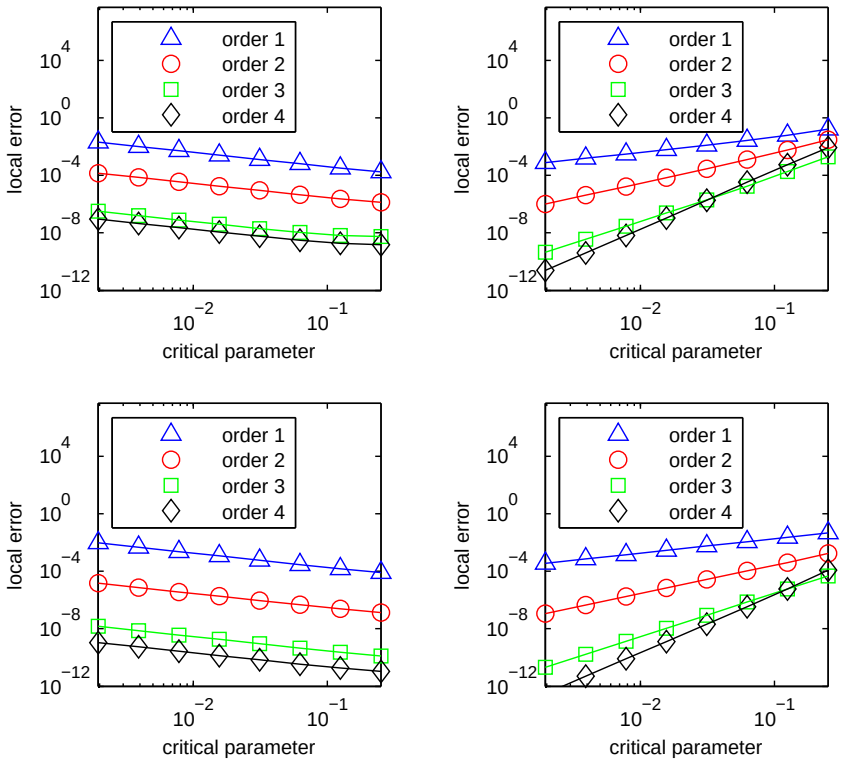

Fig. 4.1 Dependence of the local error on the critical parameter for different splitting methods applied to problem (4.2) under the initial condition (4.3) with $\omega = 1$ and $\vartheta = 1$ (top) or $\vartheta = 0$ (bottom), respectively, and $M = 4096$. Local error versus critical parameter for time step $h = 10^{-2}$ (left) and $h = \varepsilon$ (right).

numerical computation as well as the theoretical considerations. We point out that in the numerical example it is essential to ensure a high spatial resolution in order to observe the expected dependence on the critical parameter; for a one-dimensional problem, using an implementation in MATLAB, the computation time of Figure 4.1, e.g., on a standard notebook[1] amounts to a few seconds (only).

Throughout, we denote by $C > 0$ a generic constant, possibly taking different values at different occurrences. As usual, the Lebesgue space $L^2(\Omega) = L^2\big(\Omega, \mathbb{C}\big)$ of square integrable functions $f : \Omega \subset \mathbb{R}^d \to \mathbb{C}$ is endowed with inner product $(\cdot|\cdot)_{L^2}$ and corresponding norm $\|\cdot\|_{L^2}$, given by

$$(f|g)_{L^2} = \int_\Omega f(x)\,\overline{g(x)}\,\mathrm{d}x\,, \quad \big\|f\big\|_{L^2} = \sqrt{(f|f)_{L^2}}\,, \qquad f, g \in L^2(\Omega)\,. \tag{4.1a}$$

The Sobolev space $H^m(\Omega)$ comprises all functions with partial derivatives up to order $m \geq 0$ contained in $L^2(\Omega)$, where in particular $H^0(\Omega) = L^2(\Omega)$; the associated

[1] hp Compaq nc8430, Intel(R) Core(TM)2 CPU, T7200 @ 2 GHz, 1.99 GHz, 2 GB RAM

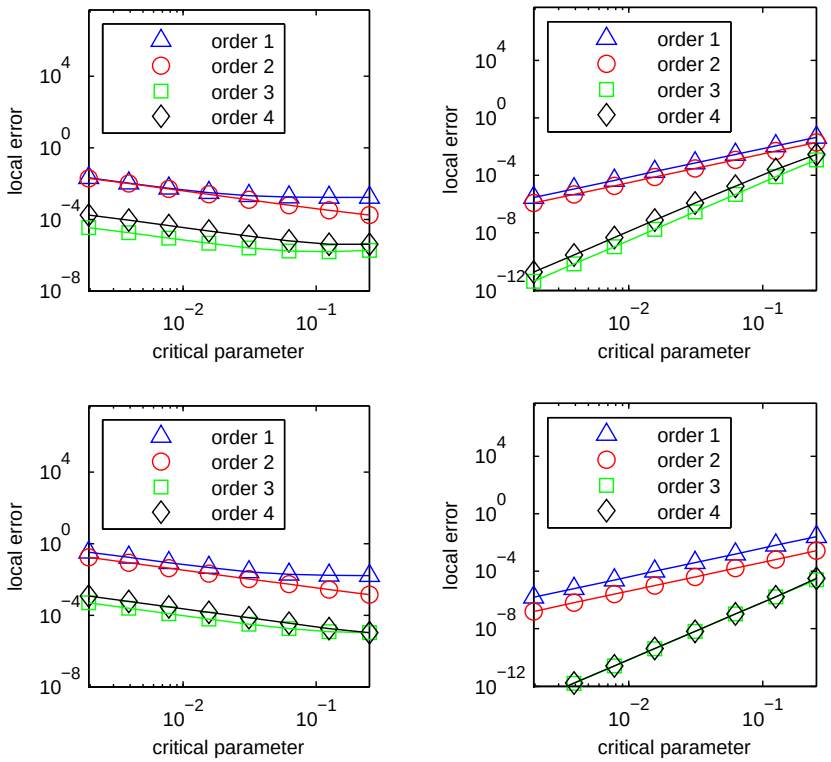

Fig. 4.2 Dependence of the local error on the critical parameter for different splitting methods applied to problem (4.2) under the initial condition (4.4) with $\omega = 1$ and $\vartheta = 1$ (top) or $\vartheta = 0$ (bottom), respectively, and $M = 4096$. Local error versus critical parameter for time step $h = 5 \cdot 10^{-2}$ (top left) or $h = 2 \cdot 10^{-1}$ (bottom left), respectively, and time step $h = \varepsilon$ (right).

norm $\|\cdot\|_{H^m}$ is defined through

$$\|f\|_{H^m}^2 = \sum_{\substack{j=(j_1,\ldots,j_d)\in\mathbb{N}^d \\ j_1+\cdots+j_d\leq m}} \|\partial^j f\|_{L^2}^2 , \qquad f \in H^m(\Omega) . \tag{4.1b}$$

Detailed information on Sobolev spaces is found in the monograph [1].

4.1 Numerical example

In the following, we illustrate the local error behaviour of higher-order exponential operator splitting methods when applied to the one-dimensional Gross–Pitaevskii equation under an initial condition in classical Wentzel–Kramers–Brillouin form and a regular initial condition, respectively; in particular, we study the dependence of the local error on the time stepsize and the critical parameter. Our model problem conforms to [4, Example 6].

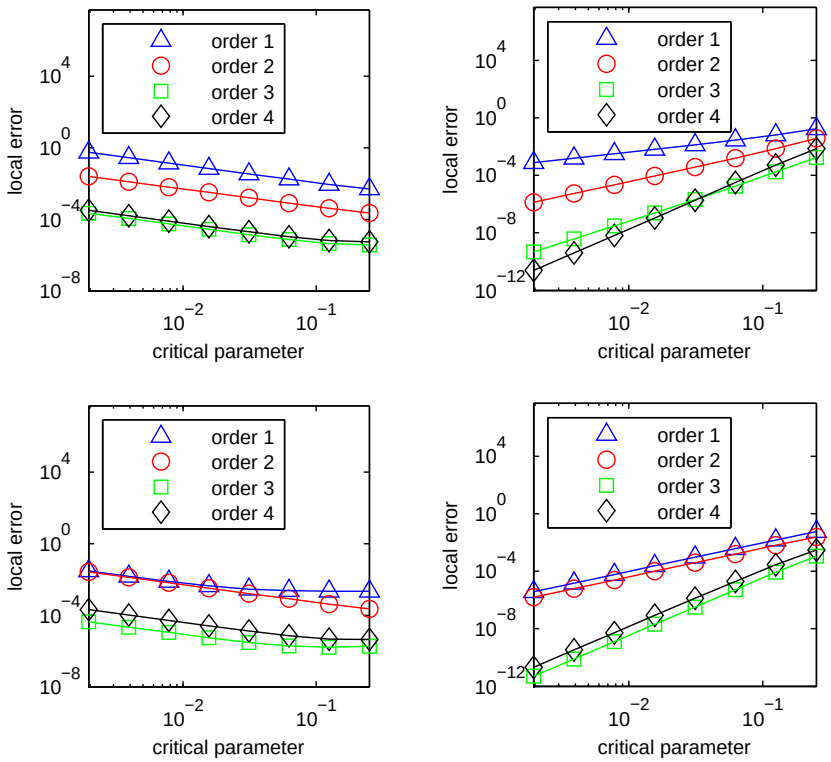

Fig. 4.3 Dependence of the local error on the critical parameter for different splitting methods applied to problem (4.2) under the initial condition (4.3) (top) or (4.4) (bottom), respectively, with $\omega = 0$, $\vartheta = 1$, and $M = 4096$. Local error versus critical parameter for time step $h = 5 \cdot 10^{-2}$ (left) and $h = \varepsilon$ (right).

Henceforth, we consider the time-dependent nonlinear Schrödinger equation

$$\begin{cases} \mathrm{i}\,\partial_t \psi(x,t) = \Big(-\frac{1}{2}\,\varepsilon\,\partial_{xx} + \frac{1}{\varepsilon}\,U(x) + \frac{1}{\varepsilon}\,\vartheta\,\big|\psi(x,t)\big|^2 \Big)\,\psi(x,t)\,, \\ \psi(x,0) = \rho_0(x)\,\mathrm{e}^{\mathrm{i}\,\sigma_0(x)/\varepsilon}\,, \qquad x \in \Omega\,, \quad 0 \le t \le T\,, \end{cases} \tag{4.2a}$$

for a function $\psi : \Omega \times [0,T] \to \mathbb{C} : (x,t) \mapsto \psi(x,t)$, where $\Omega \subset \mathbb{R}$ denotes a (suitably chosen) bounded interval. For the following, we assume the external real potential $U : \Omega \to \mathbb{R}$ and the functions $\rho_0, \sigma_0 : \Omega \to \mathbb{R}$ defining the initial condition to be sufficiently often differentiable with bounded derivatives. In particular, we study (4.2a) under a scaled harmonic potential

$$U(x) = \tfrac{1}{2}\,\omega^2 x^2\,, \qquad x \in \Omega\,, \tag{4.2b}$$

for a positive weight $\omega > 0$. In view of Section 4.2, we also consider the special case $\vartheta = 0$, where (4.2a) reduces to a linear Schrödinger equation, and the cubic Schrödinger equation, where $\omega = 0$.

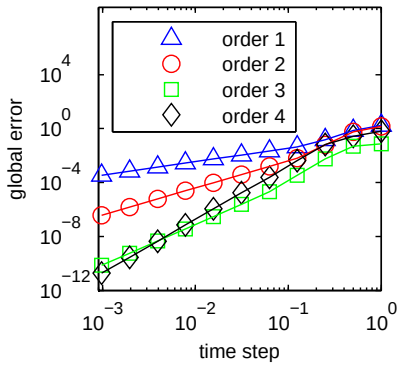

Fig. 4.4 Numerical convergence orders of different splitting methods applied to problem (4.2) under the initial condition (4.3) with $\varepsilon = 2^{-2}$, $\omega = 1$, $\vartheta = 1$, $M = 256$, and final time $T = 1$. Global error versus time stepsize.

For the numerical illustration, the values of the critical parameter $\varepsilon > 0$ are chosen in the range $2^{-9} = 1.953125 \cdot 10^{-3}$ to $2^{-2} = 2.5 \cdot 10^{-1}$. Further, we let $\omega = 1$ and $\vartheta = 1$ as well as

$$\rho_0(x) = \mathrm{e}^{-x^2}, \quad \sigma_0(x) = -\ln\left(\mathrm{e}^{x} + \mathrm{e}^{-x}\right), \qquad x \in \Omega. \tag{4.3}$$

In regard to the space discretisation by the Fourier-spectral method with $M = 4096$ degrees of freedom, we impose periodic boundary conditions on the bounded interval $\Omega = [-a, a]$; in the present situation, $a = 8$ is sufficiently large, so that the artificial boundary conditions do not cause perturbations of the numerical solution. For the time integration of (4.2), we apply exponential operator splitting methods of orders one up to four with constant time stepsize $h > 0$, namely, the first-order Lie–Trotter splitting method (2.5), the second-order Strang splitting method (2.6), a third-order splitting method with coefficients given in Table 2.1, and the fourth-order splitting method by Yoshida (2.7); on the one hand, we choose the actual time stepsize $h = h_0$ independent of the parameter ε, and, on the other hand, we set $h = \varepsilon$. Numerical reference solutions are computed by a favourable fourth-order Runge–Kutta–Nyström splitting method proposed in [6] with a finer time stepsize $h \cdot 10^{-1}$, see also Table 2.1.

In Figures 4.1 and 4.2, the local errors $\mathrm{err}_{\mathrm{local}}(\varepsilon)$ versus the critical parameter values ε are displayed, see also (3.1) for the definition of the defect; for comparison, we include the numerical results for the linear case $\vartheta = 0$ and a regular initial condition, independent of ε, namely

$$\rho_0(x) = \mathrm{e}^{-(x-\frac{1}{10})^2}, \quad \sigma_0(x) = 0, \qquad x \in \Omega, \tag{4.4}$$

as well as for the cubic Schrödinger equation, where $\omega = 0$, see Figure 4.3. In a logarithmic scale, the slopes of the lines correspond to the ratios of two subsequent local errors and parameters

$$\mathrm{ratio}(\varepsilon) = \log\left(\frac{\mathrm{err}_{\mathrm{local}}(\varepsilon)}{\mathrm{err}_{\mathrm{local}}(\varepsilon/2)}\right) / \log(2). \tag{4.5}$$

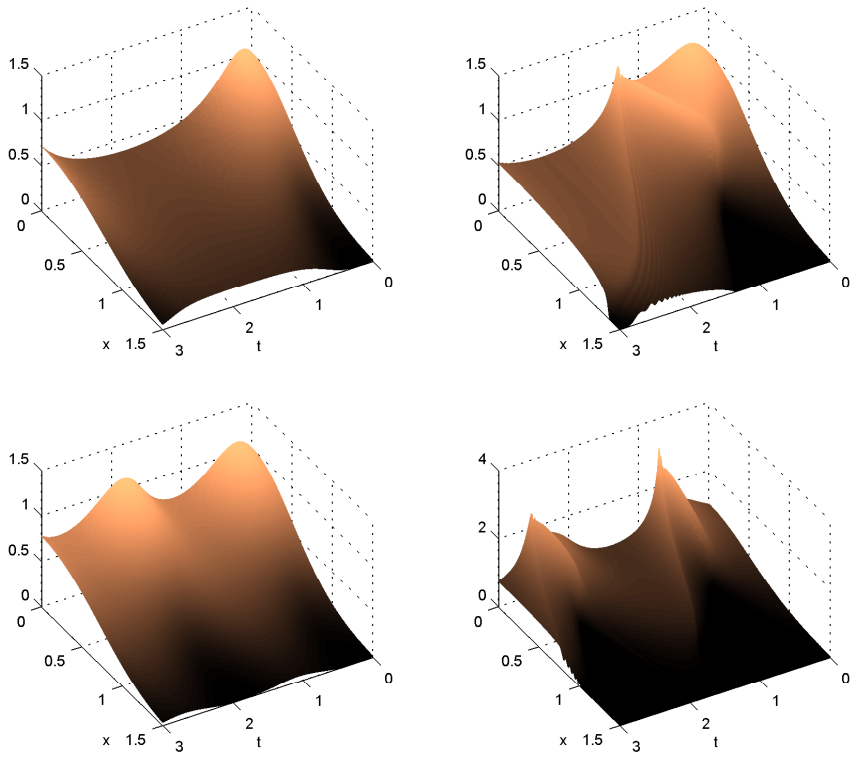

Fig. 4.5 Time evolution of the nonlinear Schrödinger equation (4.2) under the initial condition (4.3) with $\vartheta = 1$. Solution values $|\psi(x,t)|^2$, $(x,t) \in [0,1.5] \times [0,3]$, for $(\varepsilon,\omega) = (1,1)$ (top left), $(\varepsilon,\omega) = (10^{-2},1)$ (top right), $(\varepsilon,\omega) = (1,2)$ (bottom left), and $(\varepsilon,\omega) = (10^{-2},2)$ (bottom right).

For instance, for the initial condition (4.3) and a time stepsize independent of ε, it is observed that in all cases, within the chosen range of h/ε, the ratios approach the value $\alpha = -1$ which implies the dependence $\mathscr{O}(1/\varepsilon)$ of the dominant local error term with respect to the critical parameter. The numerical results are summarised in Table 4.1 and analysed in Section 4.2; thereby, $\lfloor x \rfloor$ denotes the integer part of $x \in \mathbb{R}$, i.e. $\alpha = 2\lfloor p + \frac{1}{2} \rfloor$ yields $\alpha = 2$ if $p = 1,2$, and $\alpha = 4$ if $p = 3,4$, respectively. Numerical tests not reported here show that qualitatively the same results are obtained when exchanging the roles of the operators A and B in the splitting scheme (2.4). We point out that it is crucial to choose the number of Fourier basis functions M sufficiently large to retain the expected behaviour.

As a further illustration, the global errors $\mathrm{err}_{\mathrm{global}}(h)$ at final time $T = 1$ versus the (constant) time stepsizes $h = 2^{-j}$, $0 \le j \le 10$, are displayed in Figure 4.4 for $\varepsilon = 2^{-2}$ and $M = 256$. As expected, the slopes

$$\mathrm{ratio}(h) = \log\left(\frac{\mathrm{err}_{\mathrm{global}}(h)}{\mathrm{err}_{\mathrm{global}}(h/2)}\right) / \log(2)$$

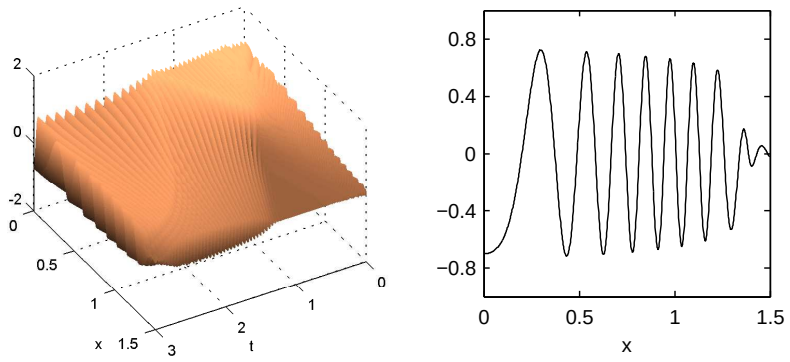

Fig. 4.6 Time evolution of the nonlinear Schrödinger equation (4.2) under the initial condition (4.3) with $\varepsilon = 10^{-2}$, $\omega = 1$, and $\vartheta = 1$. Solution values $\Re\psi(x,t)$ for $(x,t) \in [0,1.5] \times [0,3]$ (left) and section at time $t = 3$ (right).

perfectly reflect the convergence orders of the splitting methods, provided that the time stepsizes are sufficiently small; this implies the dependence $\mathscr{O}(h^{p+1})$ of the local error with respect to the time stepsize.

The time evolution of the nonlinear Schrödinger equation (4.2) with $\vartheta = 1$ under the initial condition (4.3) in classical Wentzel–Kramers–Brillouin form is illustrated in Figure 4.5. We display the solution values $|\psi(x,t)|^2$, $(x,t) \in [0,1.5] \times [0,3]$, for the parameter values $\varepsilon = 1, 10^{-2}$ and the values $\omega = 1,2$ of the constant in the confining potential; Figure 4.6 mirrors the rapid oscillations that arise for $\varepsilon = 10^{-2}$ in the graph of ψ. We choose the spatial interval $[0,1.5]$ in regard to the fact that the solution is symmetric with respect to the origin and approaches zero outside; the perspective is such that the solution values at time $t = 3$ are visible. For the space integration, we apply the Fourier-spectral method with $M = 8192$ degrees of freedom. The shape of the solution suggests an adaptive time stepsize selection; to this end, we apply the fourth-order splitting method by [6] as integrator and an embedded third-order scheme as error estimator, see Table 2.1, utilising a standard local error control as described in [16]. For absolute tolerances $\mathrm{tol} = 10^{-3j}$, $j = 1,2$, the generated time stepsize sequences which are commensurate with the solution behaviour are shown in Figures 4.7 and 4.8; in certain cases, it is needed to rigorously reduce the last timesteps to reach the final time. Furthermore, a comparison of the solution values at final time $t = 3$ is given in Figure 4.9; for $\varepsilon = 1$ both curves coincide, whereas small perturbations occur for $\varepsilon = 10^{-2}$ and $\mathrm{tol} = 10^{-3}$.

4.2 Local error estimate

In this section, we study the local error behaviour of the Lie–Trotter splitting (2.5) method for the nonlinear Schrödinger equation (4.2) in the semi-classical regime with initial condition chosen in classical Wentzel–Kramers–Brillouin form (4.3) and regular initial condition (4.4), respectively. In particular, we discuss the ability of the

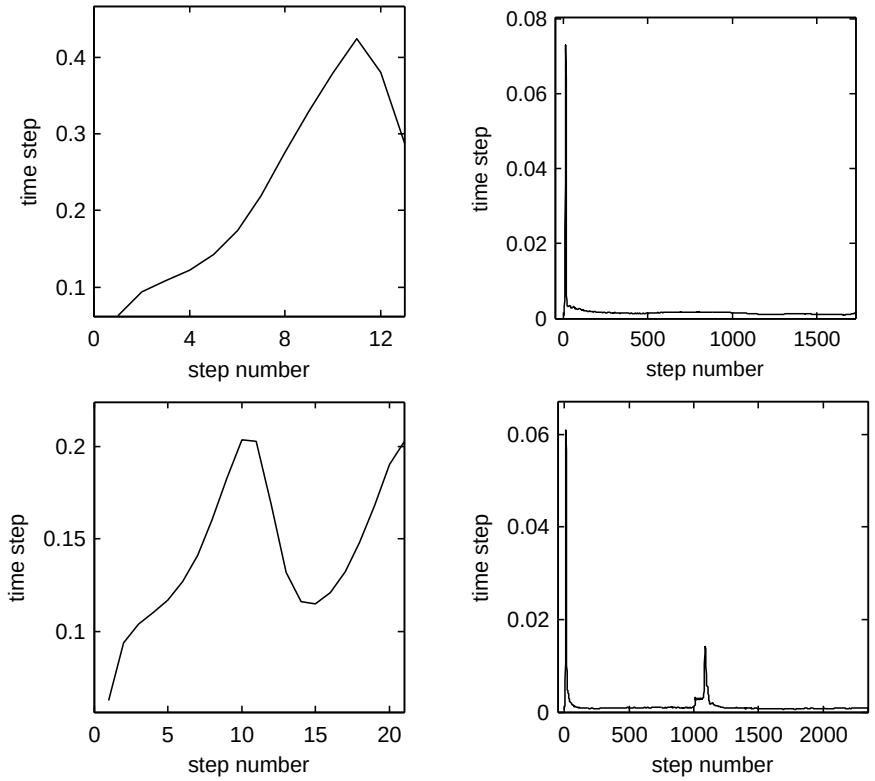

Fig. 4.7 Time evolution of the nonlinear Schrödinger equation (4.2) under the initial condition (4.3) with $\vartheta = 1$. Discretisation by the Fourier spectral method with $M = 8192$ and an embedded 4(3) time-splitting pair. Generated time stepsize sequences for an absolute tolerance of $\mathrm{tol} = 10^{-3}$ for $(\varepsilon, \omega) = (1,1)$ (top left), $(\varepsilon, \omega) = (10^{-2},1)$ (top right), $(\varepsilon, \omega) = (1,2)$ (bottom left), and $(\varepsilon, \omega) = (10^{-2},2)$ (bottom right).

exact local error representation of Theorem 1

$$\mathscr{L}(h,u_0) = \int_0^h \int_0^{\tau_1} \partial_2 \mathscr{E}_F\big(h-\tau_1, \mathscr{S}(\tau_1,u_0)\big)\, \partial_2 \mathscr{E}_B\big(\tau_1-\tau_2, \mathscr{E}_A(\tau_1,u_0)\big) \times \big[B,A\big]\Big(\mathscr{E}_B\big(\tau_2, \mathscr{E}_A(\tau_1,u_0)\big)\Big)\, \mathrm{d}\tau_2\, \mathrm{d}\tau_1 \tag{4.6}$$

to explain the dependence of the dominant local error term with respect to the actual time stepsize $h > 0$ and the critical parameter $0 < \varepsilon \ll 1$ observed numerically in Section 4.1. For the theoretical analysis, we first reconsider the linear case [10] and further the cubic Schrödinger equation, since it is then without significant difficulty to extend the arguments to the Gross–Pitaevskii equation (4.2). Concerning suitable choices of the domains of the involved operators, the computation of iterated Lie-commutators, and a possible extension to unbounded potentials in the context of the Hermite spectral method, we refer to [13,20,22,25].

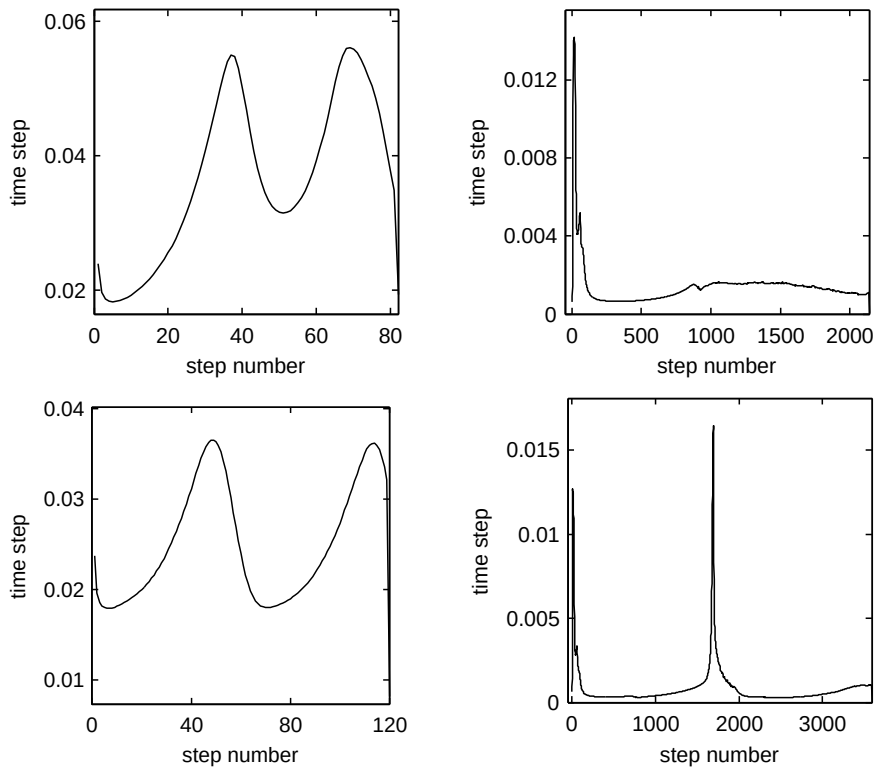

Fig. 4.8 Time evolution of the nonlinear Schrödinger equation (4.2) under the initial condition (4.3) with $\vartheta = 1$. Discretisation by the Fourier spectral method with $M = 8192$ and an embedded 4(3) time-splitting pair. Generated time stepsize sequences for an absolute tolerance of $\mathrm{tol} = 10^{-6}$ for $(\varepsilon, \omega) = (1,1)$ (top left), $(\varepsilon, \omega) = (10^{-2}, 1)$ (top right), $(\varepsilon, \omega) = (1,2)$ (bottom left), and $(\varepsilon, \omega) = (10^{-2}, 2)$ (bottom right).

The nonlinear Schrödinger equation (4.2) may be cast into the form of an abstract initial value problem (2.1) with linear operator $A : D(A) \subset X \to X$ and nonlinear operator $B : D(B) \subset X \to X$ defined by

$$A = \varepsilon \hat{A}\,, \quad \hat{A} = \tfrac{1}{2}\,\mathrm{i}\,\partial_{xx}\,, \qquad B = \tfrac{1}{\varepsilon}\,\hat{B}\,, \quad \hat{B}(v) = -\,\mathrm{i}\,\big(U + \vartheta\,|v|^2\big)\,v\,; \tag{4.7}$$

in accordance with the potential and the imposed boundary conditions on the domain $\Omega \subset \mathbb{R}$, the Sobolev embedding $H^1(\Omega) \subset L^\infty(\Omega)$ suggests suitably chosen subspaces $D(\hat{A}) \subset H^2(\Omega)$ and $D(\hat{B}) \subset H^1(\Omega)$ on the underlying Hilbert space $X = L^2(\Omega)$.

Concerning the practical realisation of a splitting method (2.4), it is favourable to rely the numerical solution of the linear subproblem

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathscr{E}_A(t,v) = A\,\mathscr{E}_A(t,v)\,, & 0 \le t \le T\,, \\ \mathscr{E}_A(0,v) = v\,, \end{cases}$$

on a spectral decomposition, see Section 4.1 and [7] for further details. Due to

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\big|\mathscr{E}_B(t,v)\big|^2 = 2\,\Re\Big(\overline{\mathscr{E}_B(t,v)}\;\tfrac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}_B(t,v)\Big) = 0\,, \qquad 0 \le t \le T\,,$$

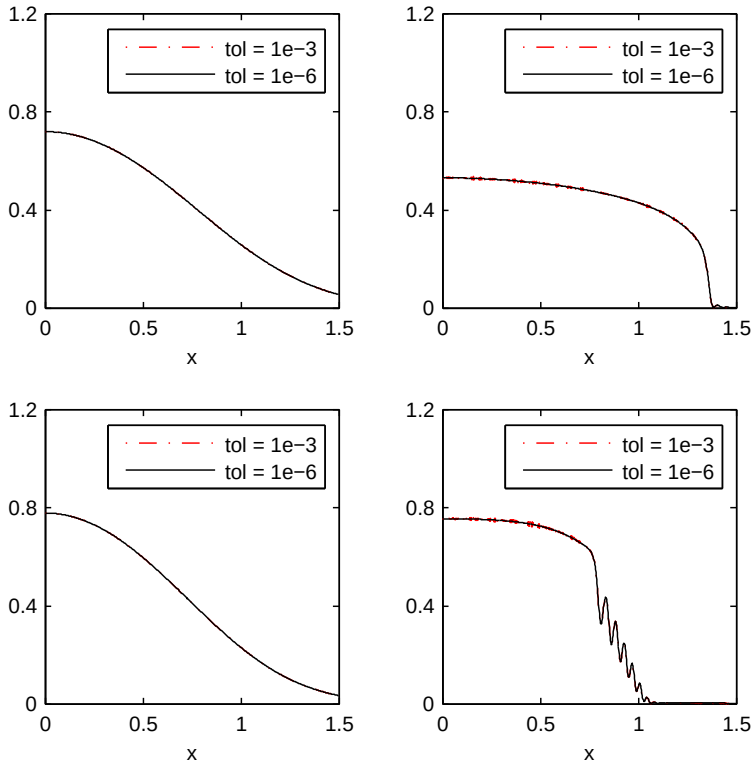

Fig. 4.9 Time evolution of the nonlinear Schrödinger equation (4.2) under the initial condition (4.3) with $\vartheta = 1$. Solution values $|\psi(x,t)|^2$, $x \in [0, 1.5]$, at time $t = 3$, computed by the Fourier spectral method with $M = 8192$ and an embedded 4(3) time-splitting pair with tolerances $\mathrm{tol} = 10^{-3j}$, $j = 1, 2$, for $(\varepsilon, \omega) = (1, 1)$ (top left), $(\varepsilon, \omega) = (10^{-2}, 1)$ (top right), $(\varepsilon, \omega) = (1, 2)$ (bottom left), and $(\varepsilon, \omega) = (10^{-2}, 2)$ (bottom right).

the invariance property $|\mathscr{E}_B(t,v)|^2 = |v|^2$, $0 \le t \le T$, follows; therefore, the analytical solution of the nonlinear subproblem

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathscr{E}_B(t,v) = B\big(\mathscr{E}_B(t,v)\big)\,, & 0 \le t \le T\,, \\ \mathscr{E}_B(0,v) = v\,, \end{cases}$$

is given in an explicit manner by

$$\mathscr{E}_B(t,v) = \mathrm{e}^{-\mathrm{i}t\,(U+\vartheta\,|v|^2)/\varepsilon}\,v\,, \qquad 0 \le t \le T\,, \tag{4.8}$$

realised numerically by a pointwise multiplication.

The Fréchet-derivatives of the linear operator $\hat{A}(v) = \hat{A}v$ and the nonlinear operator $\hat{B}(v)$ with respect to v at a point w are equal to

$$\hat{A}'(v)\,w = \hat{A}w = \tfrac{1}{2}\,\mathrm{i}\,\partial_{xx}w\,, \qquad \hat{B}'(v)\,w = -\mathrm{i}\,\big(Uw + 2\,\vartheta\,|v|^2\,w + \vartheta\,v^2\,\overline{w}\big)\,, \tag{4.9}$$

and, clearly, it holds $A' = \varepsilon\,\hat{A}'$ and $B' = \frac{1}{\varepsilon}\,\hat{B}'$, see also (4.7).

Stone's Theorem, see ENGEL AND NAGEL [11], e.g., ensures that the linear differential operator $\hat{A}$ and the nonlinear multiplication operator $\hat{B}$ generate unitary evolution operators on $L^2(\Omega)$; consequently, for any parameter value $\varepsilon > 0$ it holds

$$\big\|\mathscr{E}_A(t,\cdot)\big\|_{L^2\leftarrow L^2} = 1\,, \quad \big\|\mathscr{E}_B(t,\cdot)\big\|_{L^2\leftarrow L^2} = 1\,, \qquad 0 \le t \le T\,. \tag{4.10a}$$

Moreover, the exact solution operator is unitary on $L^2(\Omega)$, that is, the relation

$$\big\|\mathscr{E}_F(t,\cdot)\big\|_{L^2\leftarrow L^2} = 1\,, \qquad 0 \le t \le T\,, \tag{4.10b}$$

is valid; for instance, this follows from the observation that $\big(u(t)\big|\frac{\mathrm{d}}{\mathrm{d}t}u(t)\big)_{L^2} \in \mathrm{i}\mathbb{R}$ for the solution of (4.2), written in abstract form as (2.1a), wherefore

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\big\|\mathscr{E}_F\big(t,u(0)\big)\big\|_{L^2} = \tfrac{\mathrm{d}}{\mathrm{d}t}\big\|u(t)\big\|_{L^2} = 2\,\Re\big(u(t)\big|\tfrac{\mathrm{d}}{\mathrm{d}t}u(t)\big)_{L^2} = 0\,, \qquad 0 \le t \le T\,,$$

and thus the conservation property $\big\|\mathscr{E}_F\big(t,u(0)\big)\big\|_{L^2} = \|u(0)\|_{L^2}$ is valid for $0 \le t \le T$.

Clearly, it holds $\partial_2\mathscr{E}_A(t,v) = \mathscr{E}_A(t,\cdot)$ for $0 \le t \le T$ which implies that the derivative of the evolution operator $\mathscr{E}_A$ with respect to the initial value is a unitary operator on $L^2(\Omega)$. For linear Schrödinger equations, this is also valid for $\partial_2\mathscr{E}_B(t,u) = \mathscr{E}_B(t,\cdot)$ and $\partial_2\mathscr{E}_F(t,u) = \mathscr{E}_F(t,\cdot)$, $0 \le t \le T$; more generally, for nonlinear problems, the operators $\partial_2\mathscr{E}_F$ and $\partial_2\mathscr{E}_B$ satisfy the non-autonomous linear problems

$$\begin{cases} \tfrac{\mathrm{d}}{\mathrm{d}t}\,\partial_2\mathscr{E}_F(t,v) = \Big(A + B'\big(\mathscr{E}_F(t,v)\big)\Big)\,\partial_2\mathscr{E}_F(t,v)\,, \quad 0 \le t \le T\,, \\ \partial_2\mathscr{E}_F(t,v)\big|_{t=0} = I\,, \end{cases}$$

$$\begin{cases} \tfrac{\mathrm{d}}{\mathrm{d}t}\,\partial_2\mathscr{E}_B(t,v) = B'\big(\mathscr{E}_B(t,v)\big)\,\partial_2\mathscr{E}_B(t,v)\,, \quad 0 \le t \le T\,, \\ \partial_2\mathscr{E}_B(t,v)\big|_{t=0} = I\,, \end{cases}$$

with $\partial_2\mathscr{E}_B$ given explicitly by

$$\partial_2\,\mathscr{E}_B(t,v)\,w = \mathrm{e}^{-\mathrm{i}t\,(U+\vartheta\,|v|^2)/\varepsilon}\,w - 2\,\mathrm{i}\,\tfrac{t}{\varepsilon}\,\vartheta\,\mathscr{E}_B(t,v)\,\Re(\overline{v}\,w)\,, \qquad 0 \le t \le T\,, \tag{4.11}$$

see also (3.6) and (4.8).

In the following, we study the decisive term

$$\big[A,B\big](w)\,, \quad w = \mathscr{E}_B(\tau_2,v) = \mathrm{e}^{-\mathrm{i}\,\tau_2\,(U+\vartheta\,|v|^2)/\varepsilon}v\,, \quad v = \mathscr{E}_A(\tau_1,u_0)\,, \tag{4.12}$$

in the exact locar error representation (4.6). Due to the fact that

$$\begin{aligned} \hat{A}'(w)\,\hat{B}(w) &= \tfrac{1}{2}\,\partial_{xx}\big(Uw + \vartheta\,|w|^2 w\big) \\ &= \tfrac{1}{2}\,\big(U\,\partial_{xx}w + 2\,\partial_x U\,\partial_x w + \partial_{xx}U\,w + \vartheta\,w^2\partial_{xx}\overline{w} + 4\,\vartheta\,w\,|\partial_x w|^2 \\ &\qquad + 2\,\vartheta\,\overline{w}\,(\partial_x w)^2 + 2\,\vartheta\,|w|^2\partial_{xx}w\big)\,, \\ \hat{B}'(w)\,\hat{A}(w) &= \tfrac{1}{2}\,\big(U\,\partial_{xx}w + 2\,\vartheta\,|w|^2\,\partial_{xx}w - \vartheta\,w^2\,\partial_{xx}\overline{w}\big)\,, \end{aligned}$$

see (4.7) and (4.9), the first Lie-commutator of A and B is given by

$$\begin{aligned} \big[A,B\big](w) &= A'(w)\,B(w) - B'(w)\,A(w) \\ &= \hat{A}'(w)\,\hat{B}(w) - \hat{B}'(w)\,\hat{A}(w) \\ &= \partial_x U\,\partial_x w + \tfrac{1}{2}\,\partial_{xx}U w + \vartheta\,w^2\partial_{xx}\overline{w} + 2\,\vartheta\,w\,|\partial_x w|^2 + \vartheta\,\overline{w}\,(\partial_x w)^2\,, \end{aligned}$$

see (3.2); it is notable that in the nonlinear case the second spatial derivative of w arises, whereas for a linear problem (4.2) with $\vartheta = 0$ the Lie-commutator reduces to $[A,B] = \partial_x U \partial_x + \frac{1}{2}\,\partial_{xx} U\, I$, a first-order differential operator with coefficients involving the first and second derivative of the potential. A brief calculation yields

$$\begin{aligned}
\partial_x w &= \partial_x \mathrm{e}^{-\mathrm{i}\,\tau_2 (U+\vartheta\,|v|^2)/\varepsilon} v + \mathrm{e}^{-\mathrm{i}\,\tau_2 (U+\vartheta\,|v|^2)/\varepsilon} \partial_x v\,,\\
\partial_{xx} w &= \partial_{xx} \mathrm{e}^{-\mathrm{i}\,\tau_2 (U+\vartheta\,|v|^2)/\varepsilon} v + 2\,\partial_x \mathrm{e}^{-\mathrm{i}\,\tau_2 (U+\vartheta\,|v|^2)/\varepsilon} \partial_x v + \mathrm{e}^{-\mathrm{i}\,\tau_2 (U+\vartheta\,|v|^2)/\varepsilon} \partial_{xx} v\,,
\end{aligned}$$

involving the spatial derivatives

$$\begin{aligned}
\partial_x \mathrm{e}^{-\mathrm{i}\,\tau_2 (U+\vartheta\,|v|^2)/\varepsilon} &= -\mathrm{i}\,\tfrac{\tau_2}{\varepsilon}\, \mathrm{e}^{-\mathrm{i}\,\tau_2 (U+\vartheta\,|v|^2)/\varepsilon} \big(\partial_x U + 2\,\vartheta\,\Re(\overline{v}\,\partial_x v)\big)\,,\\
\partial_{xx} \mathrm{e}^{-\mathrm{i}\,\tau_2 (U+\vartheta\,|v|^2)/\varepsilon} &= \mathrm{e}^{-\mathrm{i}\,\tau_2 (U+\vartheta\,|v|^2)/\varepsilon} \Big(-\tfrac{\tau_2^2}{\varepsilon^2} \big(\partial_x U + 2\,\vartheta\,\Re(\overline{v}\,\partial_x v)\big)^2 \\
&\qquad - \mathrm{i}\,\tfrac{\tau_2}{\varepsilon} \big(\partial_{xx} U + 4\,\vartheta\,|\partial_x v|^2 + 4\,\vartheta\,\Re(\overline{v}\,\partial_{xx} v)\big)\Big)\,;
\end{aligned}$$

inserting the above relations into (4.12) thus gives

$$\begin{aligned}
\big[A,B\big](w) &= \mathrm{e}^{-\mathrm{i}\,\tau_2 (U+\vartheta\,|v|^2)/\varepsilon} \big(g_1(v) + \mathrm{i}\,\tfrac{\tau_2}{\varepsilon}\, g_2(v)\big)\,, \qquad v = \mathscr{E}_A(\tau_1, u_0)\,,\\
g_1(v) &= \partial_x U \partial_x v + \tfrac{1}{2}\,\partial_{xx} U v + \vartheta\,\partial_{xx}\overline{v} v^2 + 2\,\vartheta\,|\partial_x v|^2 v + \vartheta\,(\partial_x v)^2\,\overline{v}\,,\\
g_2(v) &= -(\partial_x U)^2 v + \vartheta\,\partial_{xx} U |v|^2 v - 2\,\vartheta\,\partial_x U\,\Re(\overline{v}\,\partial_x v)\, v\\
&\qquad + 2\,\vartheta^2\,|\partial_x v|^2 |v|^2 v + \vartheta^2\,\partial_{xx} v\,|v|^4 + \vartheta^2\,\partial_{xx}\overline{v}\,|v|^2 v^2.
\end{aligned} \tag{4.13a}$$

Provided that the linear operator A (with domain $D(A)$ also including the imposed boundary conditions) and the differential operators ∂_x commute (on a suitably chosen subdomain), it follows

$$\partial_x^j v = \mathscr{E}_A(\tau_1, \partial_x^j u_0)\,, \qquad j \geq 0\,, \tag{4.13b}$$

and further $\|\partial_x^j v\|_{L^2} = \|\partial_x^j u_0\|_{L^2}$ for $j \geq 0$, see (4.10). In particular, for initial conditions in classical Wentzel–Kramers–Brillouin form (4.3) with ρ_0 and σ_0 sufficiently often differential, we obtain

$$\begin{aligned}
u_0 &= \rho_0\, \mathrm{e}^{\mathrm{i}\,\sigma_0/\varepsilon}\,, \qquad \partial_x u_0 = \partial_x \rho_0\, \mathrm{e}^{\mathrm{i}\,\sigma_0/\varepsilon} + \tfrac{\mathrm{i}}{\varepsilon}\,\partial_x \sigma_0\, u_0\,,\\
\partial_{xx} u_0 &= \big(\partial_{xx}\rho_0 + 2\,\tfrac{\mathrm{i}}{\varepsilon}\,\partial_x \rho_0\,\partial_x \sigma_0\big)\,\mathrm{e}^{\mathrm{i}\,\sigma_0/\varepsilon} + \big(\tfrac{\mathrm{i}}{\varepsilon}\,\partial_{xx}\sigma_0 - \tfrac{1}{\varepsilon^2}\,(\partial_x \sigma_0)^2\big)\,u_0\,.
\end{aligned} \tag{4.13c}$$

In general, for $\partial_x^j \sigma_0 \neq 0$, this implies the estimate $\|\partial_x^j u_0\|_{L^2} \leq \frac{1}{\varepsilon^j} M_j$ with constant $M_j > 0$ not depending on the critical parameter ε for $j \geq 0$; especially, if $\sigma_0 = 0$, it follows $\|\partial_x^j u_0\|_{L^2} \leq M_j$ for $j \geq 0$.

Linear Schrödinger equation. For a linear Schrödinger equation, i.e., problem (4.2) with $\vartheta = 0$, the above considerations simplify to

$$\begin{gathered}
\big[A,B\big](w) = \mathrm{e}^{-\mathrm{i}\,\tau_2 U/\varepsilon} \big(g_1(v) + \mathrm{i}\,\tfrac{\tau_2}{\varepsilon}\, g_2(v)\big)\,,\\
g_1(v) = \partial_x U \partial_x v + \tfrac{1}{2}\,\partial_{xx} U v\,, \quad g_2(v) = -(\partial_x U)^2 v\,,\\
v = \mathscr{E}_A(\tau_1, u_0)\,, \quad \partial_x v = \mathscr{E}_A(\tau_1, \partial_x u_0)\,,
\end{gathered}$$

see (4.13). On the one hand, due to the fact that

$$\begin{aligned}\big\|g_1(v)\big\|_{L^2} &\leq \big\|\partial_x U\big\|_{L^\infty}\big\|\partial_x v\big\|_{L^2} + \big\|\partial_{xx} U\big\|_{L^\infty}\|v\|_{L^2}\,,\\ \big\|g_2(v)\big\|_{L^2} &\leq \big\|\partial_x U\big\|_{L^\infty}^2\|v\|_{L^2}\,,\end{aligned}$$

for initial values (4.13c) with $\sigma_0 = 0$ the bound

$$\begin{aligned}\big\|\big[A,B\big](w)\big\|_{L^2} &\leq \big\|\partial_x U\big\|_{L^\infty}\big\|\partial_x v\big\|_{L^2} + \Big(\big\|\partial_{xx} U\big\|_{L^\infty} + \tfrac{\tau_2}{\varepsilon}\,\big\|\partial_x U\big\|_{L^\infty}^2\Big)\|v\|_{L^2}\\ &\leq \big\|\partial_x U\big\|_{L^\infty}\big\|\partial_x u_0\big\|_{L^2} + \Big(\big\|\partial_{xx} U\big\|_{L^\infty} + \tfrac{\tau_2}{\varepsilon}\,\big\|\partial_x U\big\|_{L^\infty}^2\Big)\|u_0\|_{L^2}\end{aligned} \tag{4.14}$$

follows, which implies the local error estimate

$$\vartheta = 0\,,\quad \sigma_0 = 0: \qquad \big\|\mathscr{L}(h,u_0)\big\|_{L^2} \leq \big(C_0 + C_1\,\tfrac{h}{\varepsilon}\big)\,h^2$$

with constants $C_0, C_1 > 0$ involving $\|\partial_x u_0\|_{L^2}$, $\|u_0\|_{L^2}$, $\|\partial_x U\|_{L^\infty}$, and $\|\partial_{xx} U\|_{L^\infty}$, see also (4.10). Evidently, the Lie–Trotter splitting method has convergence order one, see Figure 4.4. Moreover, for a fixed time stepsize $h = h_0$ and critical parameter values $0 < \varepsilon < h$ (or, more precisely, $0 < \varepsilon < ch$ for some constant $c > 0$) the dominant local error term is $C_1 h^3/\varepsilon$ and thus the ratio $\alpha = -1$ results, whereas we obtain $\alpha = 2$ for $h = \varepsilon$, see (4.5); this is in accordance with the numerical observations summarised in Table 4.1. On the other hand, for initial values (4.13c) with first spatial derivative involving $1/\varepsilon$ (that is, $\|\partial_x u_0\|_{L^2} \leq \frac{1}{\varepsilon} M_1$), the bound (4.14) yields

$$\vartheta = 0\,,\quad \partial_x\sigma_0 \neq 0: \qquad \big\|\mathscr{L}(h,u_0)\big\|_{L^2} \leq \big(C_0\,h + C_1\,\tfrac{h}{\varepsilon}\big)\,h\,,$$

provided that $0 < h < 1$; similarly to before, for ratios h/ε where the local error term $C_1 h^2/\varepsilon$ dominates, we retain $\alpha = -1$ for $h = h_0$, but $\alpha = 1$ for $h = \varepsilon$, both confirming the numerical results given in Table 4.1.

Cubic Schrödinger equation. For the cubic Schrödinger equation, i.e., problem (4.2) with $\omega = 0$, it is more involved to deduce a local error estimate.

In regard to the regular initial condition (4.4), see also (4.13c) and let $\sigma_0 = 0$, we first suppose the initial value u_0 and thus $v = \mathscr{E}_A(\tau_1, u_0)$ to be sufficiently regular with derivatives bounded by a constant, independent of ε. We note that the following considerations could be made rigorous and that sufficient regularity requirements on u_0 are obtained by means of the Sobolev embedding $H^1(\Omega) \subset L^\infty(\Omega)$; however, as we are primarily concerned with the dependence of the local error on the time stepsize and the critical parameter, we do not specify the regularity assumptions on the initial value and the precise form of the constants. Setting $U = 0$ in (4.2), the relations in (4.13) reduce to

$$\begin{aligned}\big[A,B\big](w) &= \mathrm{e}^{-\mathrm{i}\,\tau_2\,\vartheta\,|v|^2/\varepsilon}\,\big(g_1(v) + \mathrm{i}\,\tfrac{\tau_2}{\varepsilon}\,g_2(v)\big)\,,\\ g_1(v) &= \vartheta\,\partial_{xx}\overline{v}\,v^2 + 2\,\vartheta\,|\partial_x v|^2 v + \vartheta\,(\partial_x v)^2\,\overline{v}\,,\\ g_2(v) &= 2\,\vartheta^2\,|\partial_x v|^2|v|^2 v + \vartheta^2\,\partial_{xx} v\,|v|^4 + \vartheta^2\,\partial_{xx}\overline{v}\,|v|^2 v^2\,,\\ v = \mathscr{E}_A(\tau_1,u_0)\,,&\quad \partial_x v = \mathscr{E}_A(\tau_1,\partial_x u_0)\,,\quad \partial_{xx} v = \mathscr{E}_A(\tau_1,\partial_{xx} u_0)\,.\end{aligned} \tag{4.15}$$

ε	h/ε	$\mathrm{err}_{\mathrm{local}}(\varepsilon)$	$\mathrm{ratio}(\varepsilon)$
5.00000000000e-1	1.250e-1	3.318314040129623e-3	-1.481542464484375e-002
2.50000000000e-1	2.500e-1	3.352566274062347e-3	-3.987567472693236e-002
1.25000000000e-1	5.000e-1	3.446522721795372e-3	-1.370712693825387e-001
6.25000000000e-2	1.000e+0	3.790039267831324e-3	-3.789477377625659e-001
3.12500000000e-2	2.000e+0	4.928540679180661e-3	-6.987314614573381e-001
1.56250000000e-2	4.000e+0	7.999401116445972e-3	-8.998641518757462e-001
7.81250000000e-3	8.000e+0	1.492600476861661e-2	-9.725874814930025e-001
3.90625000000e-3	1.600e+1	2.929014902784553e-2	-9.927998706142481e-001
1.95312500000e-3	3.200e+1	5.828866680385411e-2	-9.974626176915570e-001
9.76562500000e-4	6.400e+1	1.163724799946193e-1	-9.964577528699693e-001
4.88281250000e-4	1.280e+2	2.321742025889134e-1	-9.874763693867023e-001
2.44140625000e-4	2.560e+2	4.603349719843108e-1	-9.501733704707212e-001
1.22070312500e-4	5.120e+2	8.894154215722925e-1	-7.779601700474771e-001
6.10351562500e-5	1.024e+3	1.525084832985217e+0	4.144601950283195e-001
3.05175781250e-5	2.048e+3	1.144271421143380e+0	-4.118896129108623e-001
1.52587890625e-5	4.096e+3	1.522369868884755e+0	7.193399857950300e-003
7.62939453125e-6	8.192e+3	1.514798096013354e+0	

Table 4.2 Time integration of the cubic Schrödinger equation (4.2) with $\vartheta = 1$ and $\omega = 0$ under the initial condition (4.4) by the Lie–Trotter splitting method with $h = 6.25 \cdot 10^{-2}$. Dependence of the local error on the critical parameter ε.

Therefore, assuming the initial value u_0 to satisfy suitable regularity requirements such that the quantities $g_1(v)$ and $g_2(v)$ remain bounded in $L^2(\Omega)$, the estimate

$$\big\| \big[A,B\big](w) \big\|_{L^2} \le C_0 + C_1 \tfrac{h}{\varepsilon}$$

follows. The identity $\partial_2 \mathscr{E}_B(t,v)\, z = \mathrm{e}^{-\mathrm{i}t\vartheta|v|^2/\varepsilon}\big(z - 2\mathrm{i}\,\tfrac{t}{\varepsilon}\,\vartheta\,\Re(\overline{v}z)\,v\big)$, see (4.11), yields

$$\begin{aligned}
\partial_2 \mathscr{E}_B(\tau_1-\tau_2,v)\,\big[A,B\big](w) &= G_1(v) + \tfrac{\tau_2}{\varepsilon}\,G_2(v) + \tfrac{\tau_1-\tau_2}{\varepsilon}\,G_3(v) + \tfrac{(\tau_1-\tau_2)\tau_2}{\varepsilon^2}\,G_4(v)\,,\\
G_1(v) &= \mathrm{e}^{-\mathrm{i}\,\tau_1\vartheta|v|^2/\varepsilon} g_1(v)\,, \qquad G_2(v) = \mathrm{i}\,\mathrm{e}^{-\mathrm{i}\,\tau_1\vartheta|v|^2/\varepsilon} g_2(v)\,,\\
G_3(v) &= -2\,\mathrm{i}\,\vartheta\,\mathrm{e}^{-\mathrm{i}\,(\tau_1-\tau_2)\vartheta|v|^2/\varepsilon}\,\Re\big(\mathrm{e}^{-\mathrm{i}\,\tau_2\vartheta|v|^2/\varepsilon}\,g_1(v)\,\overline{v}\big)\,v\,,\\
G_4(v) &= -2\,\mathrm{i}\,\vartheta\,\mathrm{e}^{-\mathrm{i}\,(\tau_1-\tau_2)\vartheta|v|^2/\varepsilon}\,\Re\big(\mathrm{i}\,\mathrm{e}^{-\mathrm{i}\,\tau_2\vartheta|v|^2/\varepsilon}\,g_2(v)\,\overline{v}\big)\,v\,,
\end{aligned} \tag{4.16}$$

and further implies the estimate

$$\big\| \partial_2 \mathscr{E}_B(\tau_1-\tau_2,v)\,\big[A,B\big](w) \big\|_{L^2} \le C_0 + C_1\tfrac{h}{\varepsilon} + C_2\tfrac{h^2}{\varepsilon^2}\,.$$

With the help of the variation-of-constants formula, see also Theorem 2, and a Gronwall inequality, the bound $\|\partial_2 \mathscr{E}_F(t,v)\|_{L^2\leftarrow L^2} \le C\,(1+\tfrac{h}{\varepsilon})$ results, and, as a consequence, we finally obtain the local error estimate

$$U=0\,,\quad \sigma_0 = 0: \qquad \big\| \mathscr{L}(h,u_0) \big\|_{L^2} \le \big(C_0 + C_1\tfrac{h}{\varepsilon} + C_2\tfrac{h^2}{\varepsilon^2} + C_3\tfrac{h^3}{\varepsilon^3}\big)\,h^2$$

with constants $C_j > 0$ for $0 \le j \le 3$. The above bound shows that for a fixed time stepsize $h = h_0$ the size of the ratio h/ε (as well as the size of the involved constants) determines the dominant local error term. Indeed, for ratios h/ε relatively small the

term $C_0 h^2$ dominates, whereas for h/ε large the dominant term is $C_3 h^5/\varepsilon^3$. Figure 4.3 and further numerical results given in Table 4.2 indicate that, in the present example, for h/ε in a certain range the local error of the Lie–Trotter splitting method is dominated by $C_1 h^3/\varepsilon$ which explains the ratio $\alpha \approx -1$ and that for h/ε exceeding a certain value the local error becomes unsatisfactorily large. On the other hand, for time stepsizes $h = \varepsilon$ the above considerations for the Lie-Trotter splitting method imply $\big\|\mathscr{L}(\varepsilon, u_0)\big\|_{L^2} \leq C\,\varepsilon^2$, that is, $\alpha \approx 2$, in accordance with the numerical example, see Table 4.1.

At first glance, the numerical results obtained for classical Wentzel–Kramers–Brillouin initial conditions (4.3), that is, for initial values (4.13c) with $\partial_x \sigma_0 \neq 0$, are astonishing. Indeed, in regard to (4.15) one would suppose that the estimate for the first Lie-commutator

$$\big\|\big[A,B\big](w)\big\|_{L^2} \leq C_0 \tfrac{1}{\varepsilon^2} + C_1 \tfrac{h}{\varepsilon^3}$$

and the resulting local error bound

$$\big\|\mathscr{L}(h, u_0)\big\|_{L^2} \leq C_0 \tfrac{h^2}{\varepsilon^2} + C_1 \tfrac{h^3}{\varepsilon^3} + C_2 \tfrac{h^4}{\varepsilon^4} + C_3 \tfrac{h^5}{\varepsilon^5}$$

are optimal with respect to the critical parameter; however, the above local error estimate is not consistent with the numerical illustrations. In the following, we give heuristic considerations that are conclusive with the numerical observations; however, it is left for future work to make these arguments rigorous. It is notable that the initial value $u_0 = \rho_0\, \mathrm{e}^{\mathrm{i}\,\sigma_0/\varepsilon}$ fulfills the relations

$$g_1(u_0) = \vartheta\, u_0\, \rho_0\, \partial_{xx}\rho_0 + 3\,\vartheta\, u_0 \big(\partial_x \rho_0\big)^2 - \tfrac{\mathrm{i}}{\varepsilon}\,\vartheta\, u_0\, \rho_0^2\, \partial_{xx}\sigma_0\,, \qquad \big\|g_1(u_0)\big\|_{L^2} \leq C\tfrac{1}{\varepsilon}\,,$$
$$g_2(u_0) = 2\,\vartheta^2\, u_0\, \rho_0^2 \big(\partial_x \rho_0\big)^2 + 2\,\vartheta^2\, u_0\, \rho_0^3\, \partial_{xx}\rho_0\,, \qquad \big\|g_2(u_0)\big\|_{L^2} \leq C\,.$$

Ignoring for a moment the effect of the evolution operator $\mathscr{E}_A$, that is, supposing that $v = \mathscr{E}_A(\tau_1, u_0)$ coincides with u_0, one would obtain $\|[A,B](w)\|_{L^2} \leq C_0 \frac{1}{\varepsilon} + C_1 \frac{h}{\varepsilon}$. Evidently, the above simplification is not satisfied in general, but, as we conjecture from calculations based on a stepwise expansion in the lines of

$$v = \mathscr{E}_A(\tau_1, u_0) = u_0 + \int_0^1 \tau_1 A\, \mathrm{e}^{\sigma\,\tau_1 A} u_0\, \mathrm{d}\sigma\,,$$

the following estimates are valid

$$\big\|g_1(v)\big\|_{L^2} \leq \tfrac{1}{\varepsilon}\, Q_1\big(\tfrac{h}{\varepsilon}\big)\,, \qquad \big\|g_2(u_0)\big\|_{L^2} \leq Q_2\big(\tfrac{h}{\varepsilon}\big)\,,$$

involving (convergent) power series Q_j for $j = 1, 2$. The above conjecture yields the commutator bound

$$\big\|\big[A,B\big](w)\big\|_{L^2} \leq \tfrac{1}{\varepsilon}\, Q_1\big(\tfrac{h}{\varepsilon}\big) + \tfrac{h}{\varepsilon}\, Q_2\big(\tfrac{h}{\varepsilon}\big)\,,$$

and, regarding (4.16) and $\|\partial_2 \mathscr{E}_F(t,v)\|_{L^2 \leftarrow L^2} \leq C(1 + \frac{h}{\varepsilon})$, we further obtain the local error estimate

$$U = 0\,, \quad \partial_x \sigma_0 \neq 0: \qquad \big\|\mathscr{L}(h, u_0)\big\|_{L^2} \leq Q\big(\tfrac{h}{\varepsilon}\big)\, h\,, \quad Q(\xi) = \sum_{j=0}^{\infty} C_j\, \xi^j\,,$$

which conforms to the numerical results, see also Table 4.1. In fact, for a fixed time stepsize $h = h_0$ the ratio h/ε determines the dominant local error term; in the numerical example, the dominant term is $C_1 h^2/\varepsilon$. On the other hand, for $h = \varepsilon$ the ratio $\alpha \approx 1$ is observed.

Gross–Pitaevskii equation. Altogether, the above considerations for the linear Schrödinger equation and the cubic Schrödinger equation imply the following local error estimate for the Lie-Trotter splitting method (2.5) when applied to the Gross–Pitaevskii equation (4.2) in the semi-classical regime, see also (2.1a), provided that the functions ρ_0 and σ_0 defining the initial condition (4.13c) satisfy suitable regularity requirements. In case of a regular initial condition (4.4), for time stepsizes $0 < h < 1$ and parameter values $0 < \varepsilon < 1$ the local error estimate

$$\sigma_0 = 0 : \qquad \big\| \mathscr{L}(h, u_0) \big\|_{L^2} \leq P\big(\tfrac{h}{\varepsilon}\big)\, h^2 , \quad P(\xi) = \sum_{j=0}^{3} C_j \, \xi^j , \tag{4.17}$$

is valid; on the other hand, we conjecture that the bound

$$\partial_x \sigma_0 \neq 0 : \qquad \big\| \mathscr{L}(h, u_0) \big\|_{L^2} \leq Q\big(\tfrac{h}{\varepsilon}\big)\, h , \quad Q(\xi) = \sum_{j=0}^{\infty} C_j \, \xi^j ,$$

holds for initial conditions in classical Wentzel–Kramers–Brillouin form (4.3). We note that the first bound is rigorous, whereas it remains to fill in the blank in the latter; both local error estimates are consistent with the numerical examples given in Section 4.1.

5 Conclusions

The present work is a further attempt to contribute to the study of exponential operator splitting methods for nonlinear evolution equations; our main concern is to expose the derivation of an exact local error representation that is well-suited in the presence of unbounded nonlinear operators and critical parameters and its analysis within the context of nonlinear Schrödinger equations in the semi-classical regime. Such a local error representation is of relevance from a theoretical and a practical perspective; it is an essential ingredient in the convergence analysis of splitting methods for nonlinear evolution equations and provides the basis for an adaptive time stepsize selection, which is indispensable in the numerical solution of complex practical applications.

Throughout, as we hoped to thereby enhance clarity, general comprehensibility, and readability, we focused on the first-order Lie–Trotter splitting method and considered as model problem the time-dependent Gross–Pitaevskii equation in a single space dimension [4, Example 6], both involving marginal technicalities. Our central theme is to demonstrate that, contrary to other approaches, our exact local error representation is conclusive with the error behaviour observed in the numerical example. Our conclusion is that in case of a regular initial condition with bounded spatial derivatives, independent of the critical parameter $0 < \varepsilon \ll 1$, time stepsizes of

the magnitude of ε are needed, whereas for an initial condition in classical Wentzel–Kramers–Brillouin form time stepsizes sufficiently smaller than the critical parameter are required. For comparison and as an incentive for future work, we further included numerical experiments that confirm the expectation that higher-order exponential operator splitting methods possess improved accuracy properties. Furthermore, we illustrate the capability of a local time stepsize control, which permits to achieve reliable numerical results by the specification of the local error tolerance.

A rigorous treatment of higher-order exponential operator splitting methods applied to general problem classes such as nonlinear evolutionary Schrödinger equations or nonlinear parabolic problems, respectively, is the objective of future work. As indicated, the (formal) extension of Theorem 1 to general splitting methods by means of the calculus of Lie-derivatives seems to be straightforward. Moreover, it is expected that a generalisation of the error estimate (4.17) relies on the techniques employed in Section 4.2; however, it seems to be more involved to provide a rigorous error analysis incorporating classical Wentzel–Kramers–Brillouin initial conditions.

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